

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051823\
 Data File : BF133440.D
 Acq On : 18 May 2023 16:07
 Operator : CG\JU
 Sample : 02828-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3

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: BF133440.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.898	473	478	492	rVB	965630	1290464	20.24%	2.963%
2	5.328	547	551	562	rBV	4659016	4764690	74.74%	10.942%
3	5.716	614	617	621	rBV	94944	82403	1.29%	0.189%
4	6.363	722	727	730	rBV	4766290	4697164	73.68%	10.787%
5	6.710	783	786	791	rBV	1413602	1095486	17.18%	2.516%
6	7.281	878	883	886	rBV	3534575	3073326	48.21%	7.058%
7	7.998	1001	1005	1008	rBV	1818421	1531677	24.03%	3.517%
8	9.075	1184	1188	1191	rBV	6571043	5597637	87.81%	12.855%
9	9.751	1299	1303	1306	rBV	2052320	1789010	28.06%	4.108%
10	10.463	1418	1424	1428	rBV	407339	344828	5.41%	0.792%
11	10.539	1433	1437	1440	rBV	3856273	3491719	54.77%	8.019%
12	10.910	1493	1500	1505	rBV7	40503	75971	1.19%	0.174%
13	11.233	1551	1555	1558	rBV	2278501	1883980	29.55%	4.326%
14	11.769	1641	1646	1665	rBV2	1009255	1421145	22.29%	3.264%
15	12.145	1704	1710	1712	rBV3	71930	129742	2.04%	0.298%
16	12.557	1774	1780	1790	rBV	368438	576603	9.05%	1.324%
17	12.645	1790	1795	1802	rVB	91756	185098	2.90%	0.425%
18	12.821	1820	1825	1828	rBV	6349885	6374800	100.00%	14.639%
19	12.845	1828	1829	1838	rVB	313785	220925	3.47%	0.507%
20	13.416	1921	1926	1933	rVB4	85521	188833	2.96%	0.434%
21	13.745	1975	1982	1996	rBV4	227593	630140	9.88%	1.447%
22	13.868	1997	2003	2009	rVV	1847763	1705412	26.75%	3.916%
23	14.010	2024	2027	2031	rBV2	82479	132105	2.07%	0.303%
24	14.345	2081	2084	2089	rVB2	84251	93667	1.47%	0.215%
25	14.521	2109	2114	2119	rBV	91528	159774	2.51%	0.367%
26	14.645	2132	2135	2141	rVB2	70822	72217	1.13%	0.166%
27	14.715	2144	2147	2153	rVB	98600	105418	1.65%	0.242%
28	14.963	2186	2189	2194	rVB	70147	79291	1.24%	0.182%
29	15.027	2196	2200	2209	rVB3	75317	142122	2.23%	0.326%
30	15.292	2240	2245	2249	rBV	1250332	1460276	22.91%	3.353%
31	15.733	2317	2320	2325	rVB2	53448	70761	1.11%	0.162%
32	16.198	2396	2399	2405	rVB3	47111	78889	1.24%	0.181%

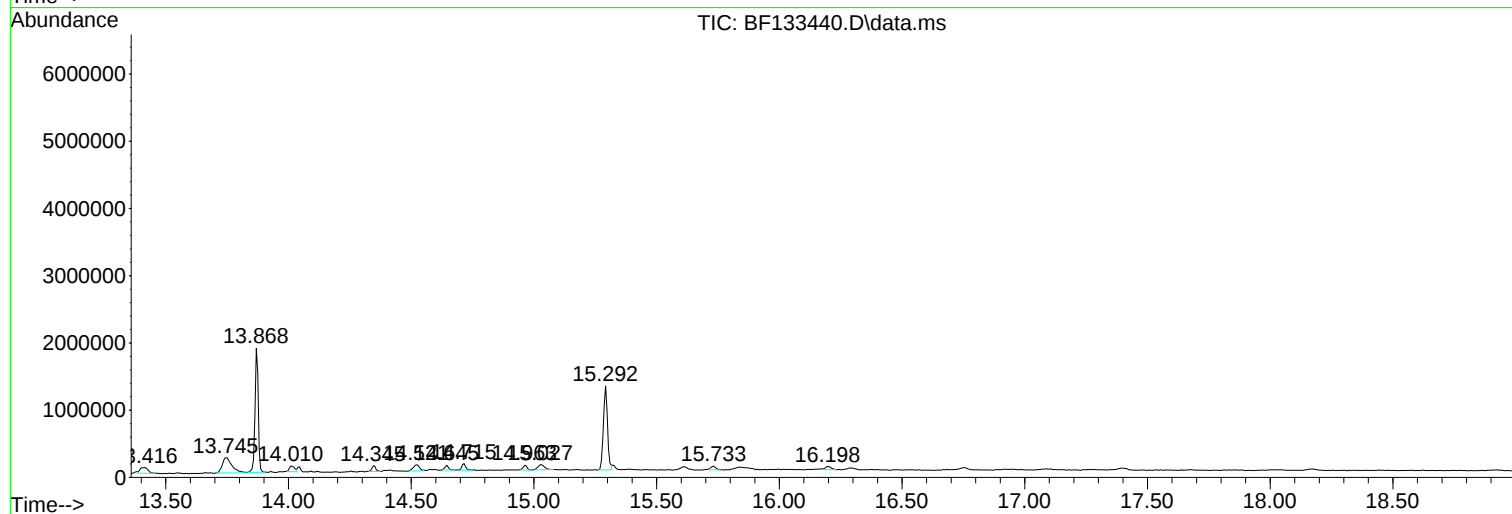
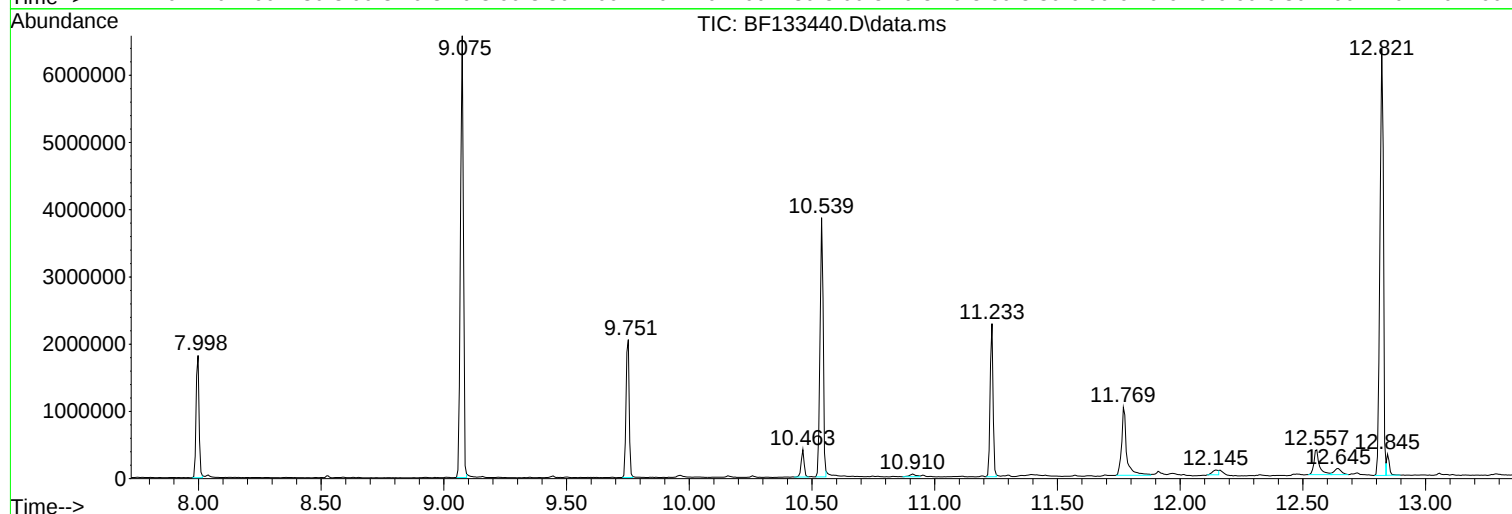
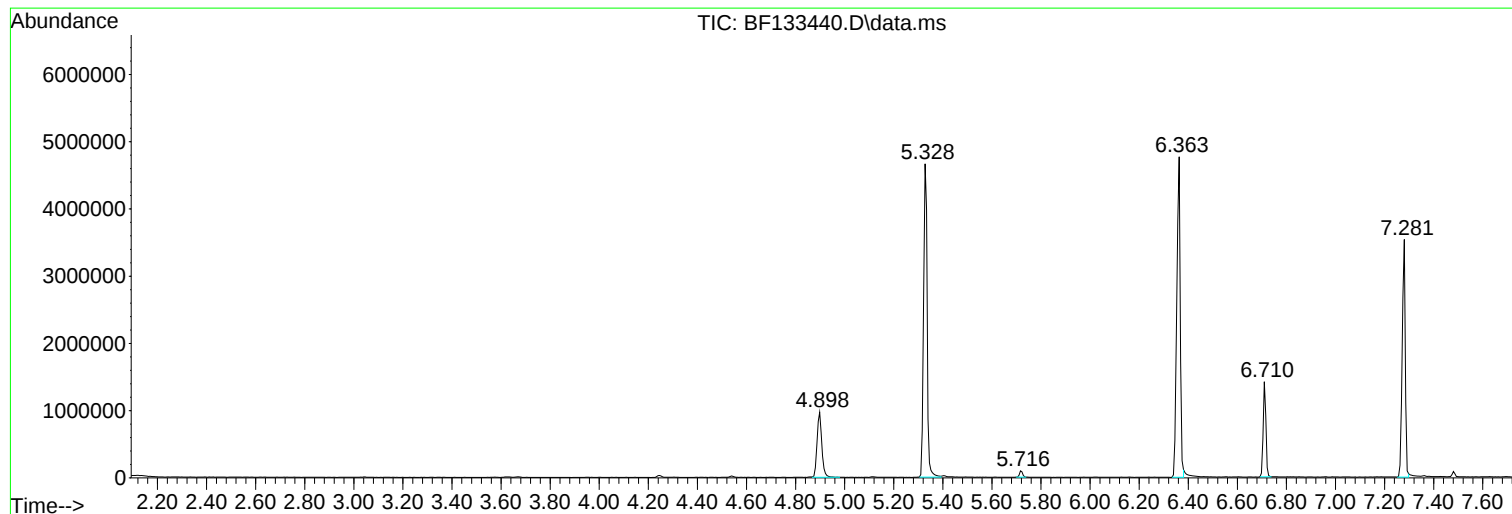
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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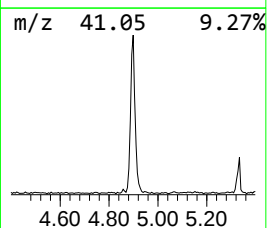
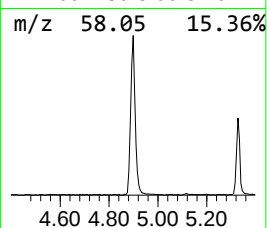
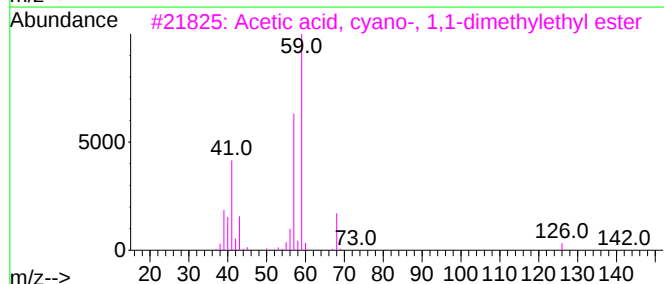
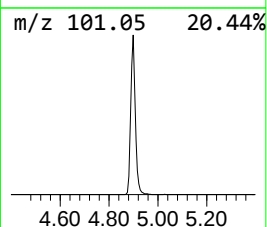
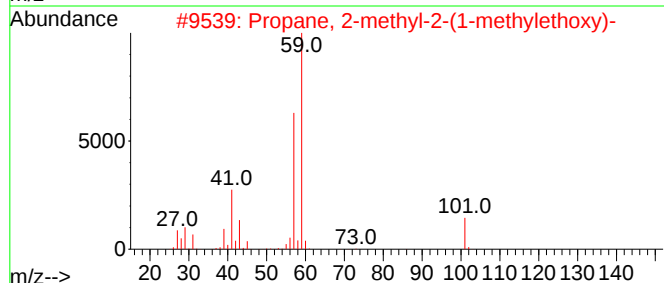
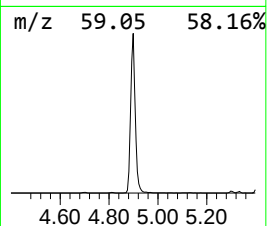
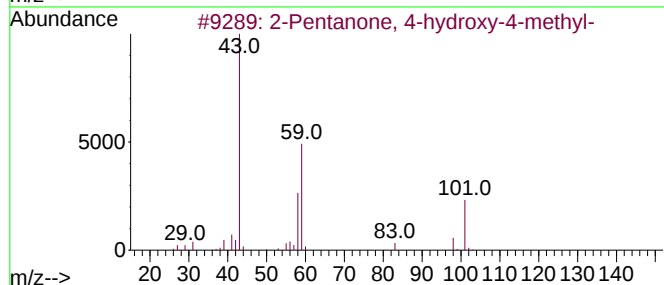
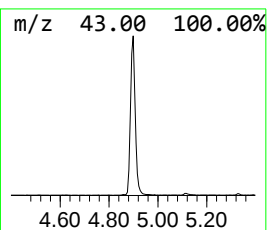
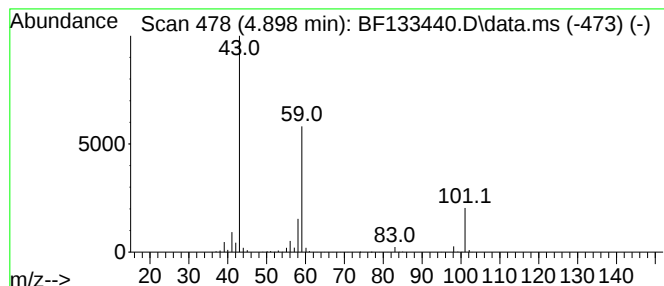
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.898	23.56 ng	1290460	1,4-Dichlorobenzene-d4	6.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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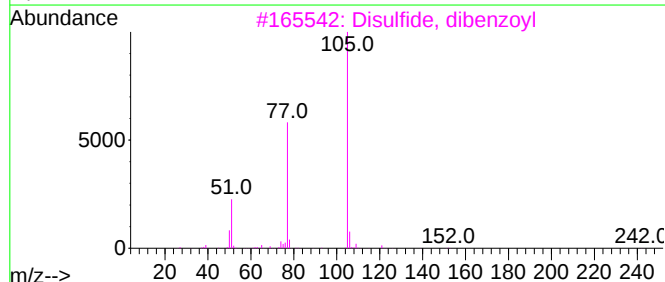
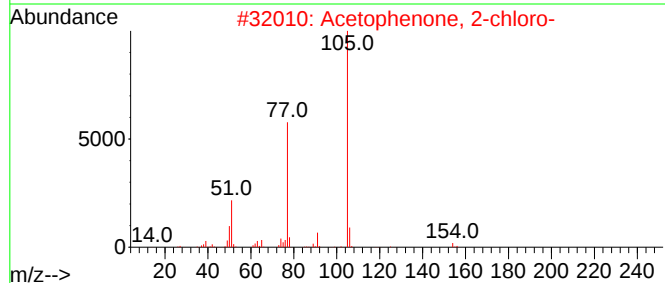
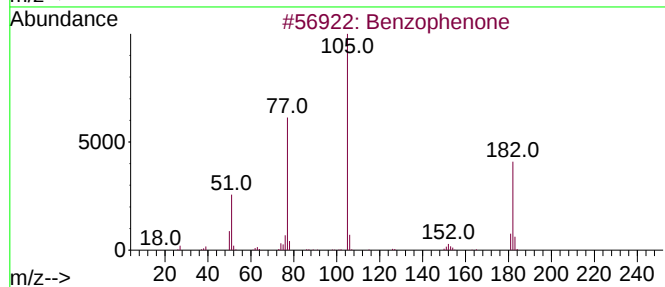
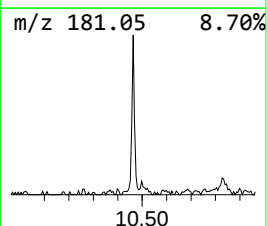
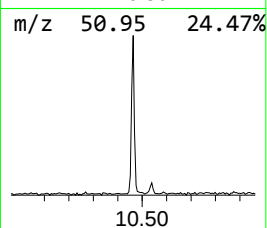
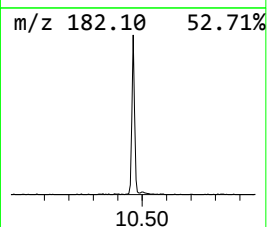
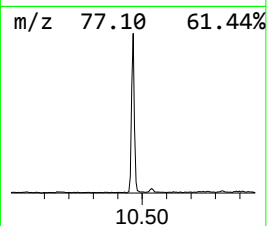
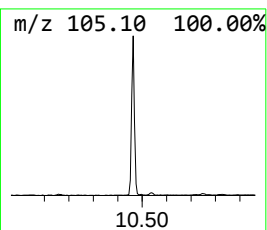
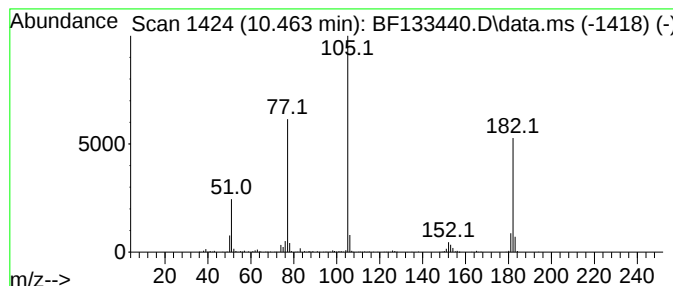
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.463	3.85 ng	344828	Acenaphthene-d10	9.751

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	53
3			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
4			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47



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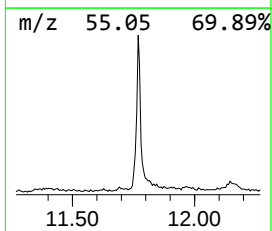
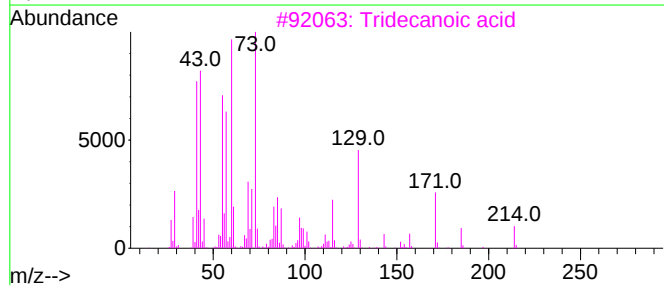
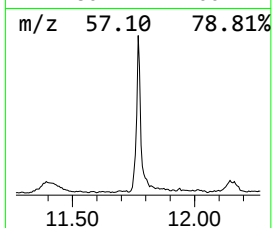
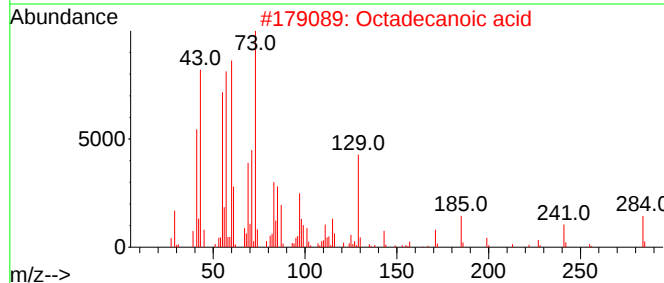
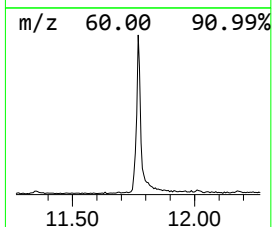
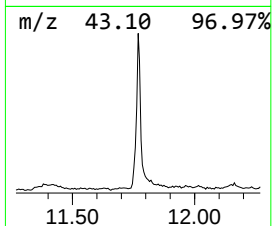
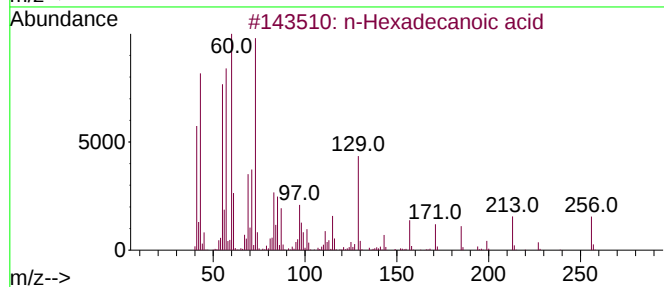
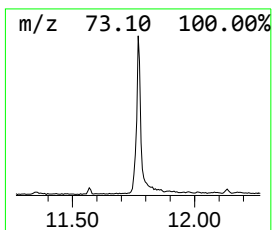
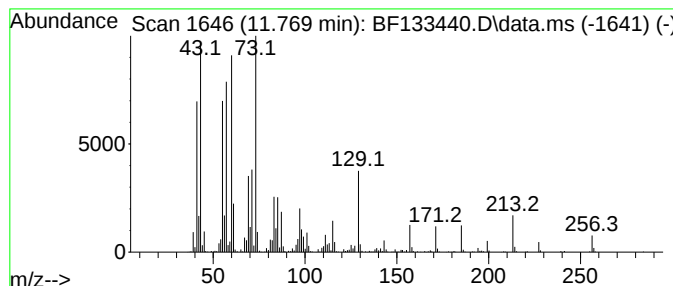
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.769	15.09 ng	1421150	Phenanthrene-d10		11.233	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Octadecanoic acid		284	C18H36O2	000057-11-4	97
3	Tridecanoic acid		214	C13H26O2	000638-53-9	91
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	87
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	80



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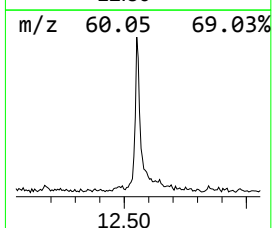
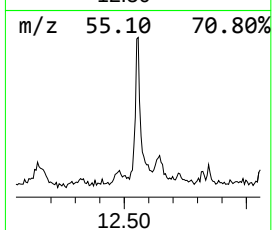
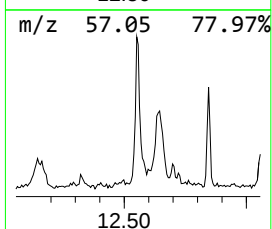
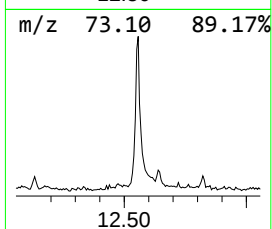
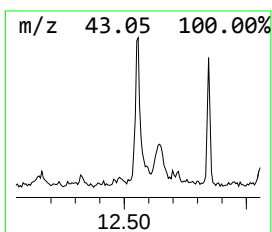
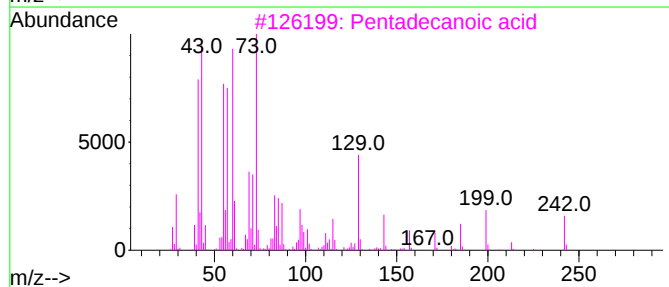
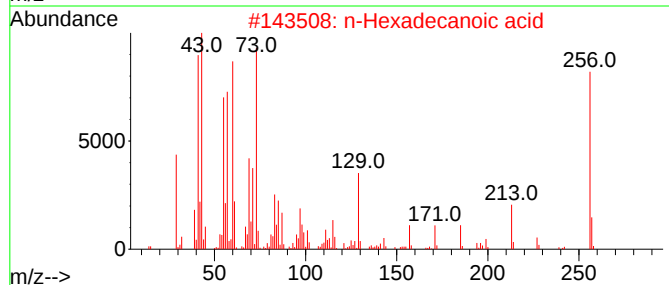
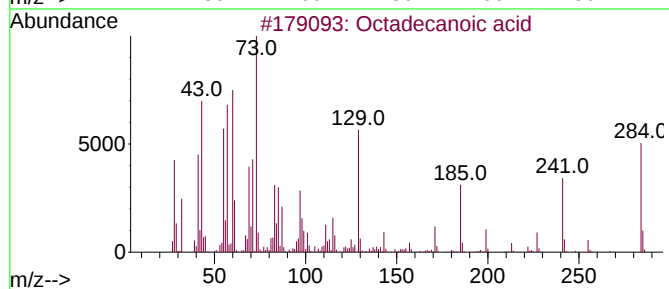
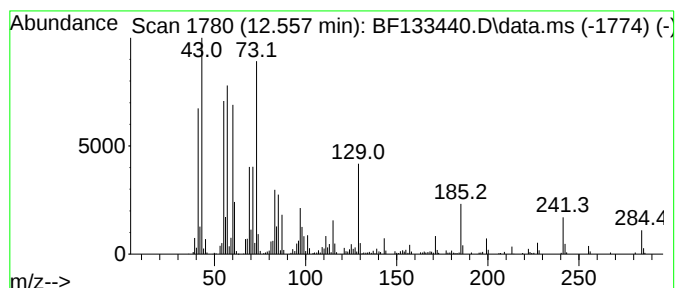
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.557	6.76 ng	576603	Chrysene-d12	13.868

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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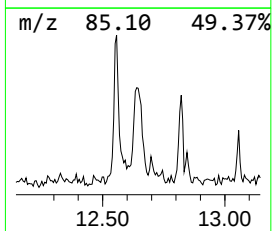
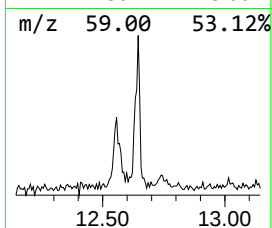
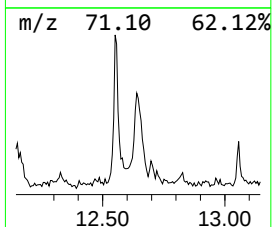
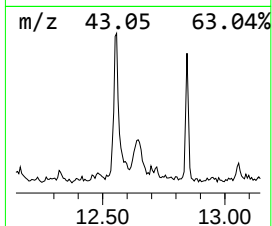
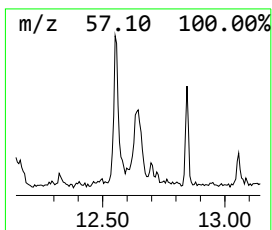
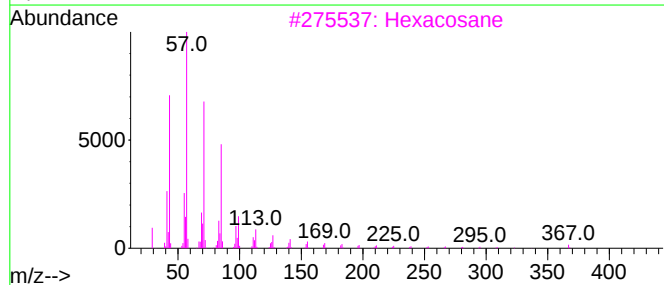
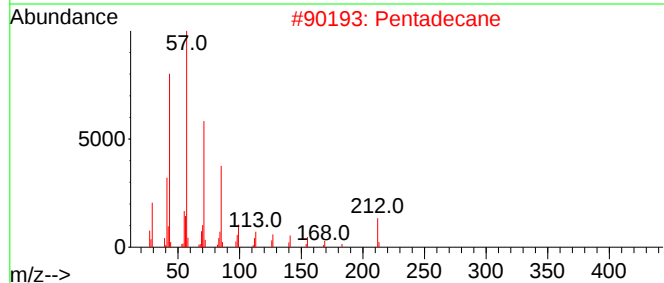
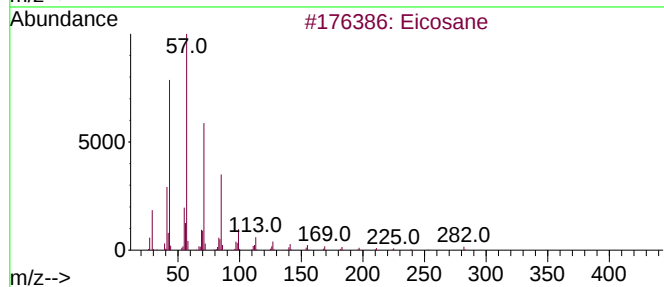
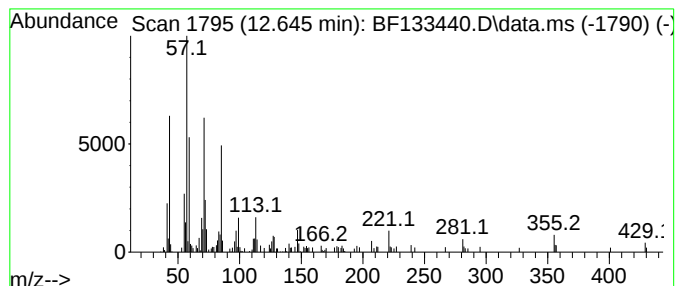
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Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	2.17 ng	185098	Chrysene-d12	13.868

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	53
2			Pentadecane	212	C15H32	000629-62-9	52
3			Hexacosane	366	C26H54	000630-01-3	50
4			Octacosane	394	C28H58	000630-02-4	45
5			Pentacosane	352	C25H52	000629-99-2	43



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SB-3

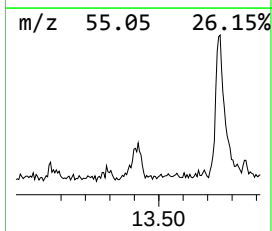
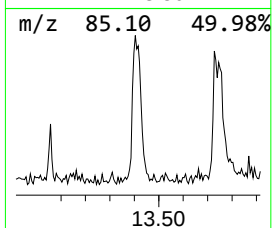
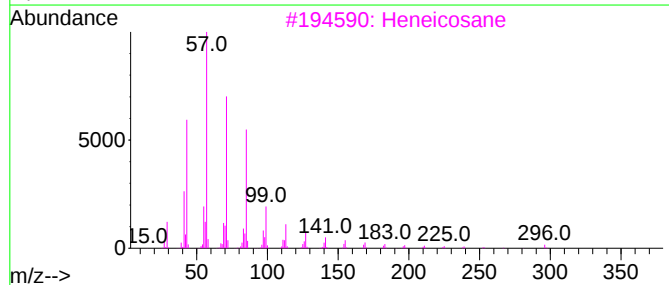
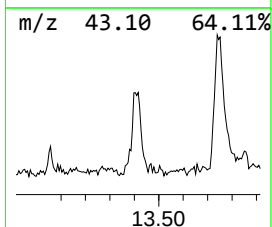
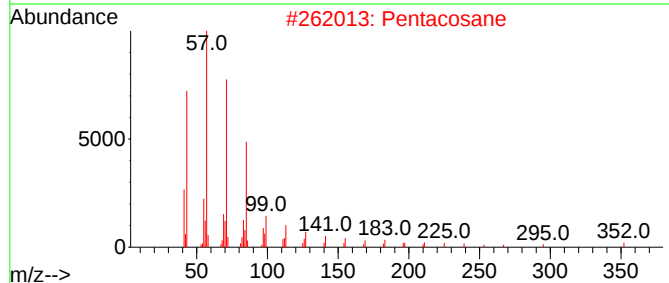
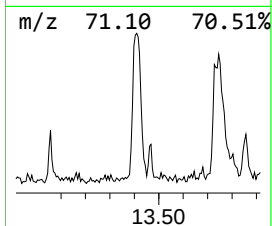
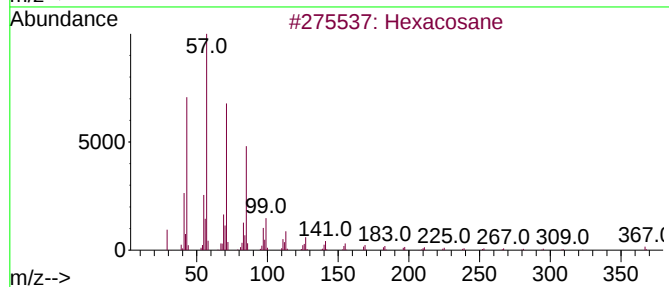
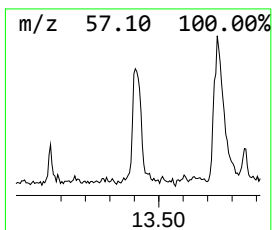
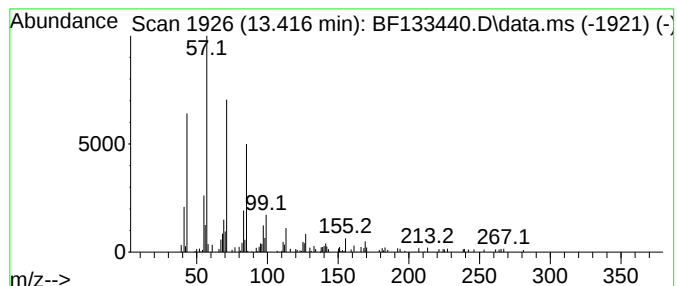
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.416	2.21 ng	188833	Chrysene-d12	13.868

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	87
2			Pentacosane	352	C25H52	000629-99-2	83
3			Heneicosane	296	C21H44	000629-94-7	83
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	80
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051823\
Data File : BF133440.D
Acq On : 18 May 2023 16:07
Operator : CG\JU
Sample : 02828-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3

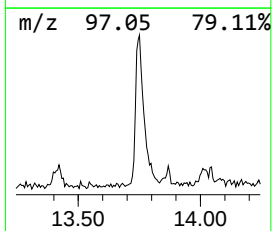
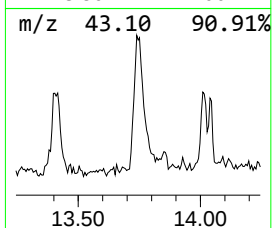
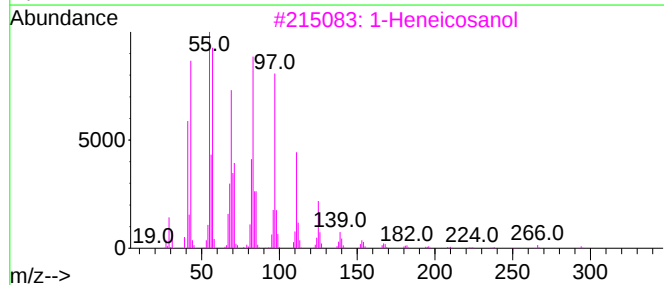
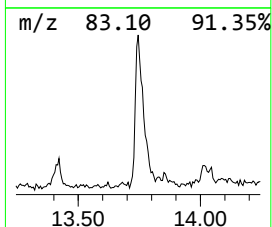
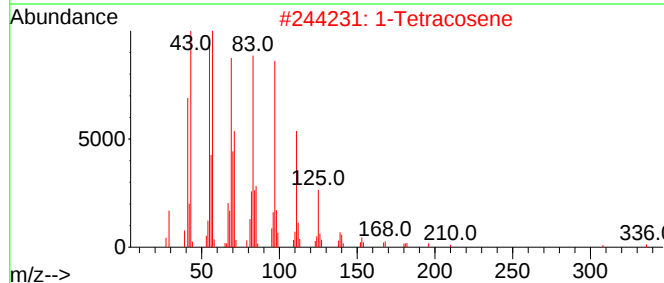
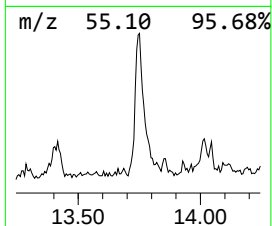
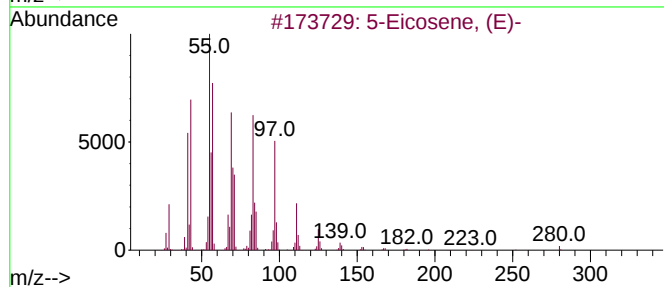
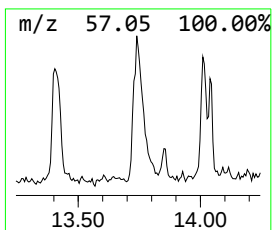
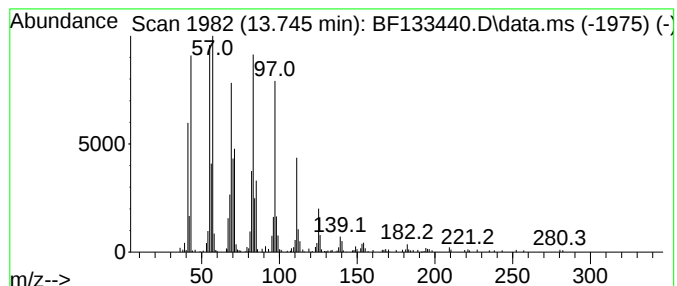
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.745	7.39 ng	630140	Chrysene-d12	13.868

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2		1-Tetracosene	336	C24H48	010192-32-2	95
3		1-Heneicosanol	312	C21H44O	015594-90-8	95
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051823\
Data File : BF133440.D
Acq On : 18 May 2023 16:07
Operator : CG\JU
Sample : 02828-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.898	23.6	ng	1290460	1	6.710	1095490	20.0
Benzophenone	10.463	3.9	ng	344828	3	9.751	1789010	20.0
n-Hexadecanoic ...	11.769	15.1	ng	1421150	4	11.233	1883980	20.0
Octadecanoic acid	12.557	6.8	ng	576603	5	13.868	1705410	20.0
Eicosane	12.645	2.2	ng	185098	5	13.868	1705410	20.0
Hexacosane	13.416	2.2	ng	188833	5	13.868	1705410	20.0
5-Eicosene, (E)-	13.745	7.4	ng	630140	5	13.868	1705410	20.0