

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121223\
 Data File : BF136527.D
 Acq On : 12 Dec 2023 21:03
 Operator : CG\JU
 Sample : 05470-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-1

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-BF120523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136527.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	14	18	24	rVB	29704	45214	1.66%	0.240%
2	5.034	496	501	512	rVB	387021	514517	18.89%	2.729%
3	5.440	565	570	573	rBV	2564062	2598117	95.37%	13.780%
4	6.439	735	740	743	rBV	2171703	2540651	93.26%	13.476%
5	6.792	797	800	804	rBV	619273	511699	18.78%	2.714%
6	7.357	891	896	899	rBV	1689476	1577124	57.89%	8.365%
7	8.069	1013	1017	1021	rBV	716274	634361	23.29%	3.365%
8	9.151	1196	1201	1204	rBV	3322499	2724137	100.00%	14.449%
9	9.827	1312	1316	1320	rBV	839145	652262	23.94%	3.460%
10	10.622	1447	1451	1454	rBV	1802997	1554767	57.07%	8.247%
11	11.322	1566	1570	1572	rBV	645854	599506	22.01%	3.180%
12	11.339	1572	1573	1577	rVB	105824	78966	2.90%	0.419%
13	11.857	1657	1661	1664	rBV	131463	130592	4.79%	0.693%
14	12.539	1773	1777	1780	rBV	143115	132955	4.88%	0.705%
15	12.645	1791	1795	1800	rBV3	43232	53366	1.96%	0.283%
16	12.763	1809	1815	1818	rBV	121830	128979	4.73%	0.684%
17	12.916	1837	1841	1844	rBV	2773741	2366311	86.86%	12.551%
18	13.463	1930	1934	1937	rBV	418629	346923	12.74%	1.840%
19	13.892	2001	2007	2015	rBV7	38973	109151	4.01%	0.579%
20	13.968	2016	2020	2023	rVV	636977	660768	24.26%	3.505%
21	13.998	2023	2025	2028	rVB	51380	40015	1.47%	0.212%
22	14.068	2034	2037	2043	rVB3	35755	45443	1.67%	0.241%
23	14.451	2099	2102	2106	rVB2	46660	43202	1.59%	0.229%
24	14.610	2126	2129	2134	rBV2	47517	46845	1.72%	0.248%
25	15.015	2195	2198	2201	rBV	40141	61073	2.24%	0.324%
26	15.409	2262	2265	2268	rVB	59197	72335	2.66%	0.384%
27	15.451	2268	2272	2277	rBV	422730	529284	19.43%	2.807%
28	15.733	2317	2320	2324	rVB3	43260	55041	2.02%	0.292%

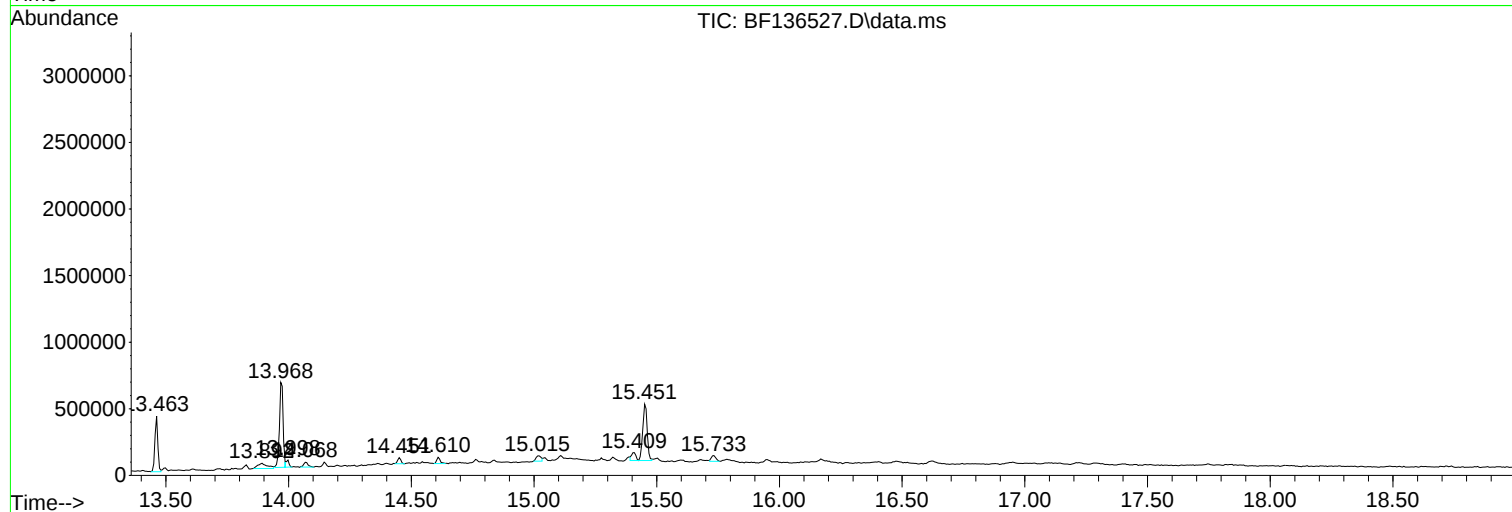
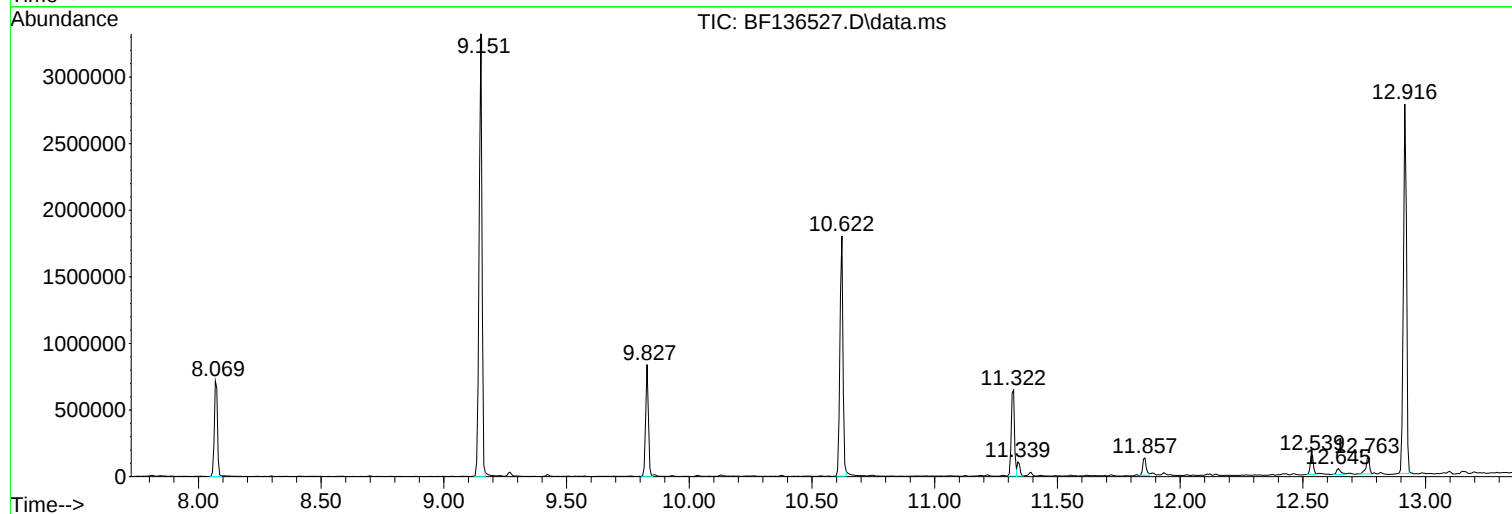
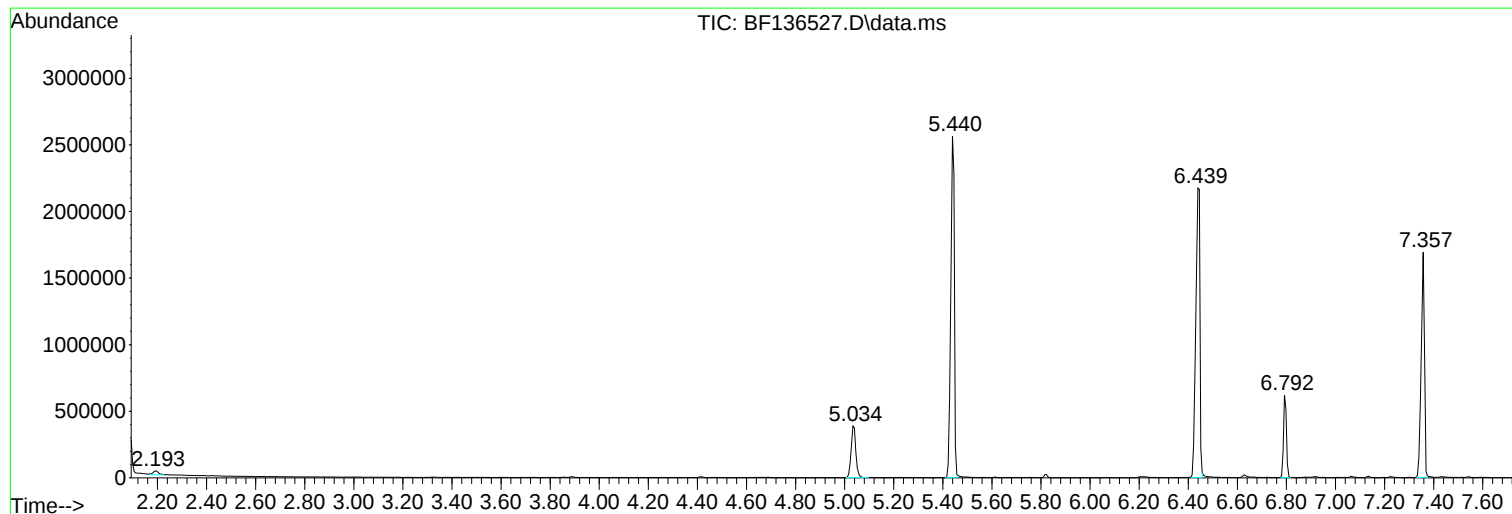
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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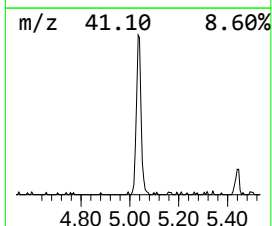
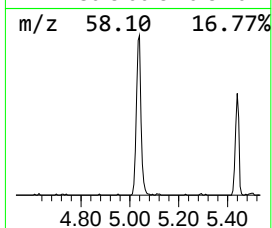
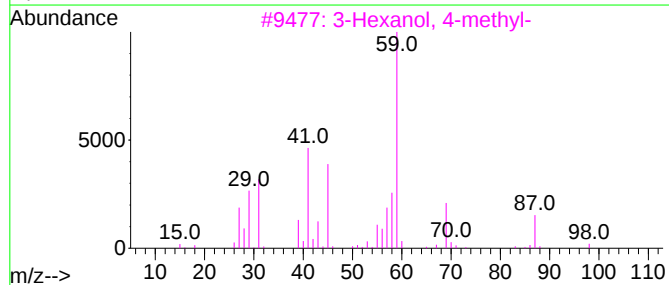
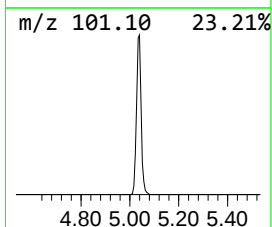
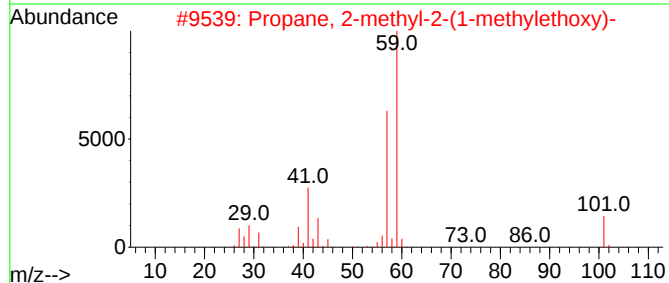
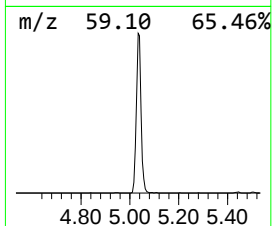
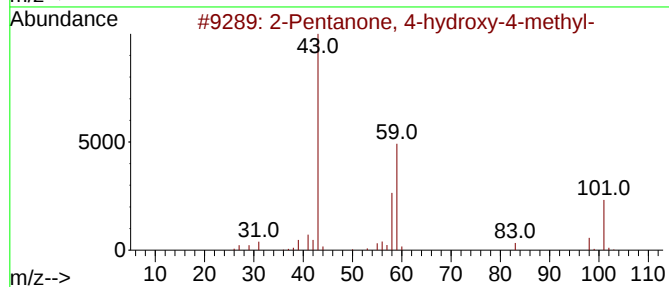
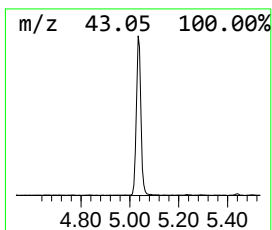
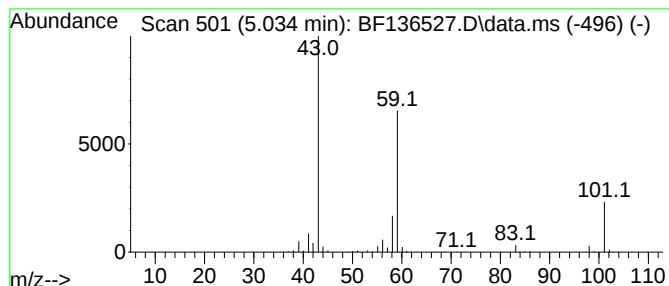
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	20.11 ng	514517	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	Guanidine	59	CH5N3	000113-00-8	9		



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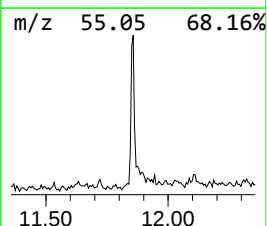
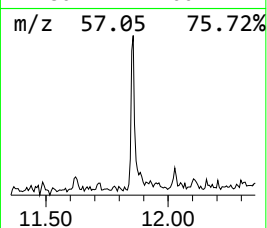
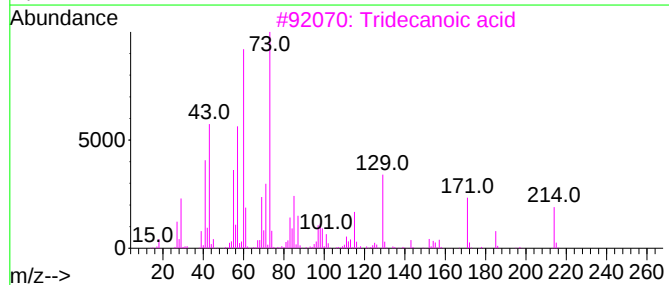
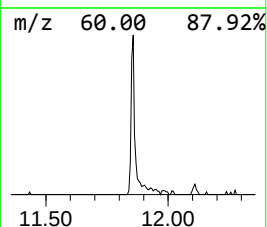
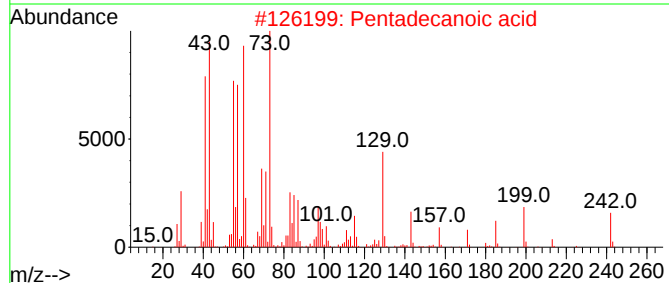
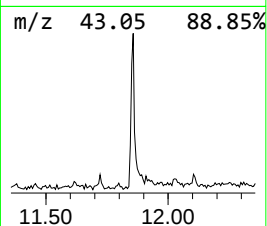
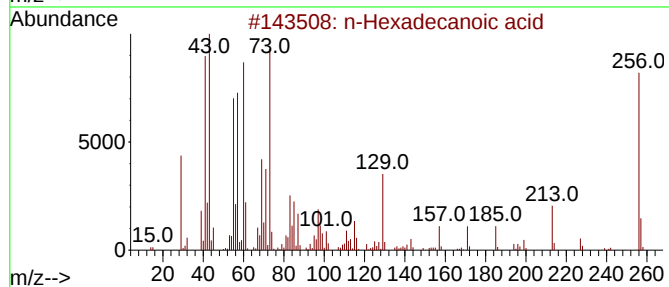
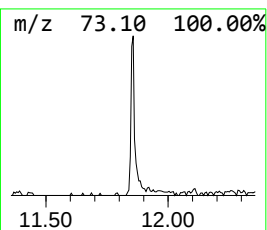
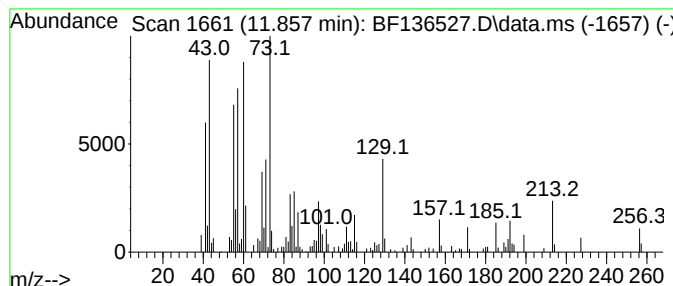
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	4.36 ng	130592	Phenanthrene-d10	11.322

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	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Undecanoic acid	186	C11H22O2	000112-37-8	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	74



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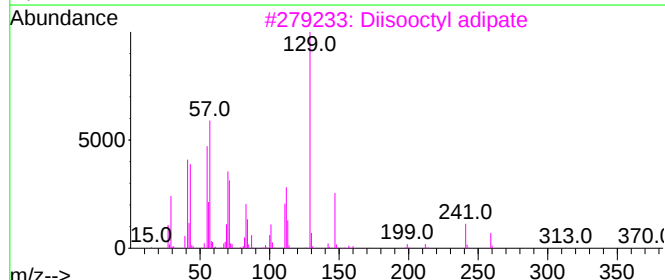
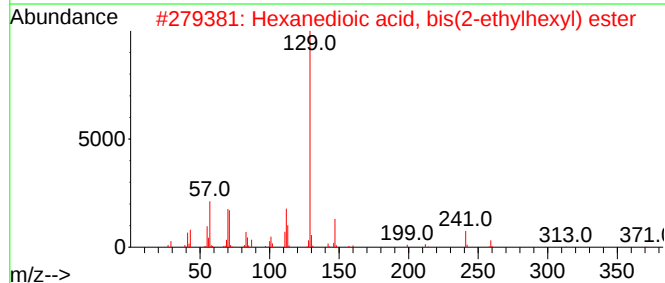
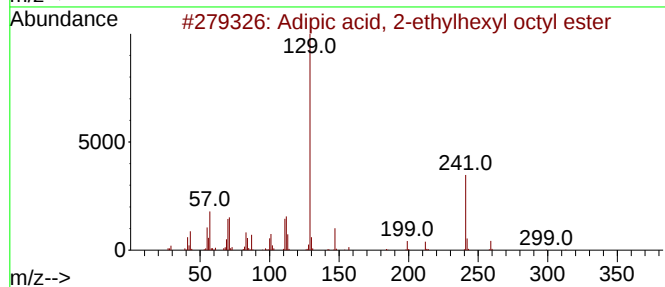
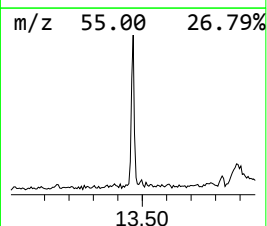
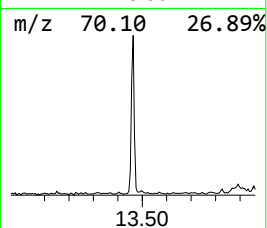
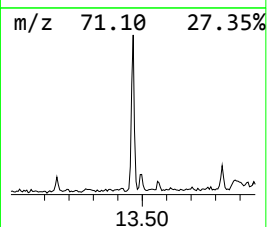
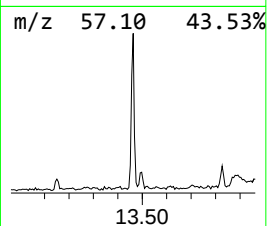
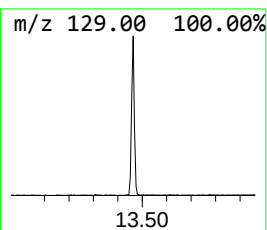
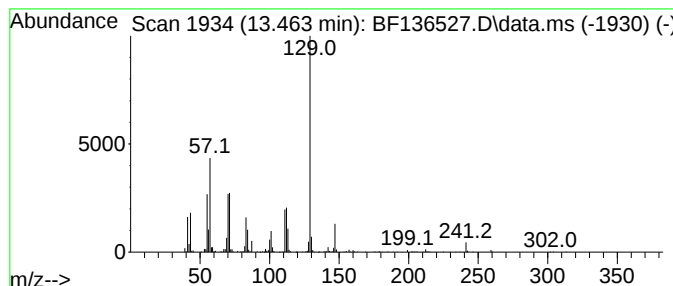
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Peak Number 3 Adipic acid, 2-ethylhexyl o... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	10.50 ng	346923	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	90
2			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	87
3			Diisooctyl adipate	370	C22H42O4	001330-86-5	78
4			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	70
5			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	50



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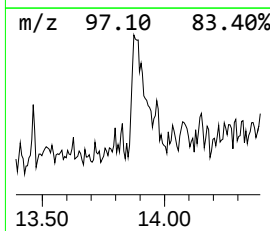
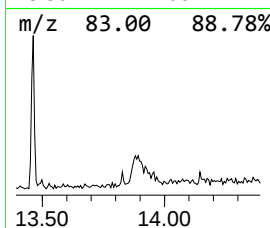
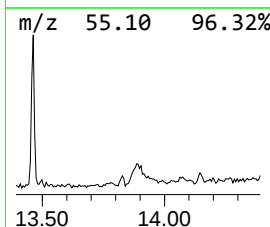
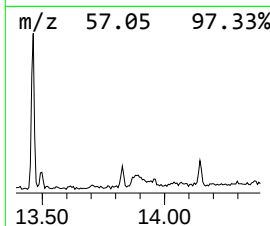
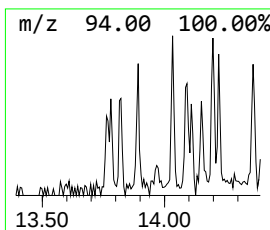
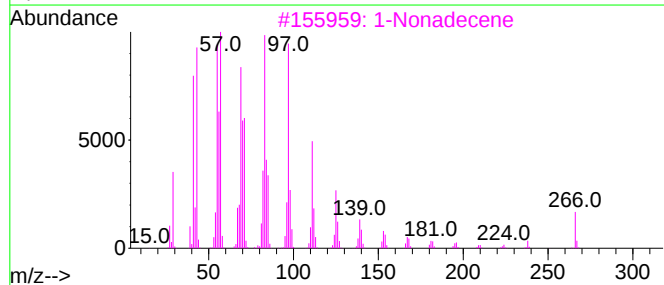
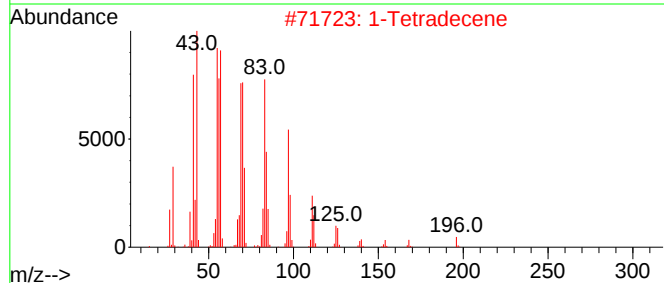
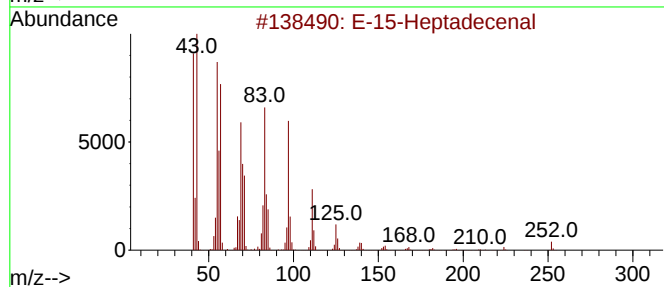
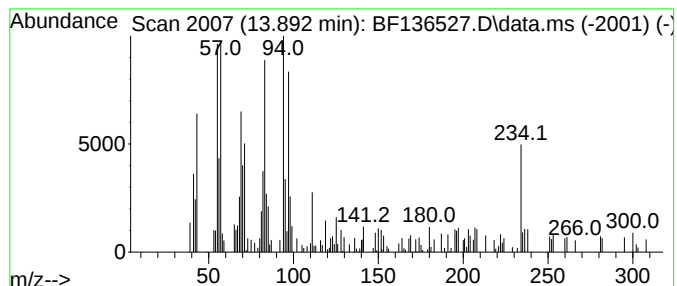
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Peak Number 4 E-15-Heptadecenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	3.30 ng	109151	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal			252	C17H32O	1000130-97-9	80
2	1-Tetradecene			196	C14H28	001120-36-1	70
3	1-Nonadecene			266	C19H38	018435-45-5	64
4	1-Octadecene			252	C18H36	000112-88-9	56
5	Cetene			224	C16H32	000629-73-2	50



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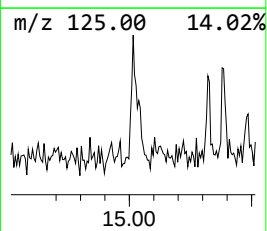
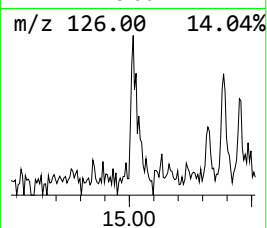
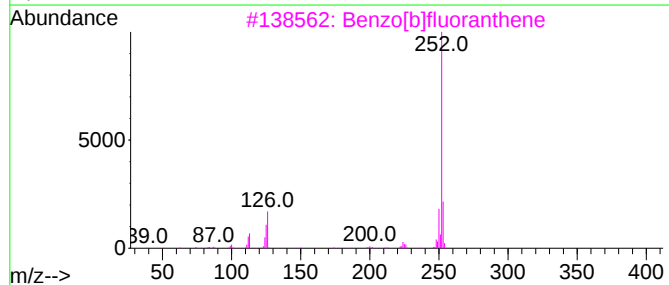
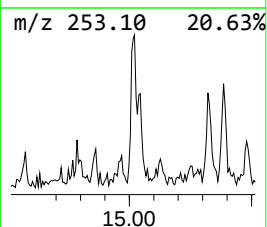
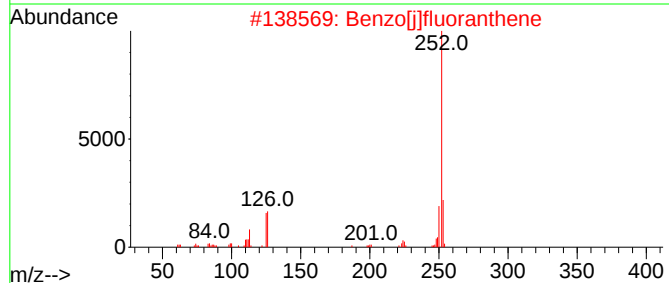
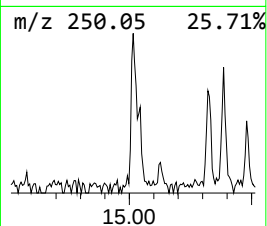
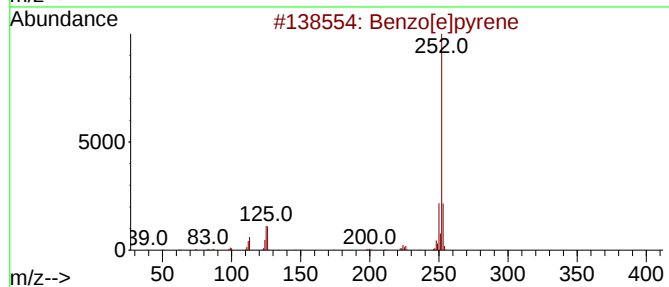
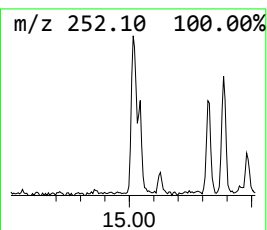
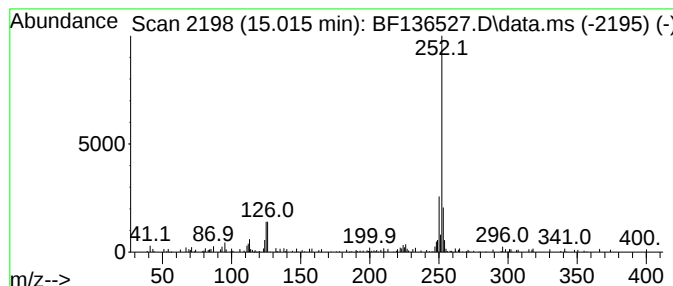
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.015	2.31 ng	61073	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	96
2			Benzo[j]fluoranthene	252	C20H12	000205-82-3	94
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4			Benzo[a]pyrene	252	C20H12	000050-32-8	91
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	91



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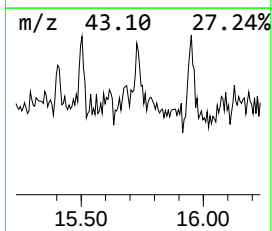
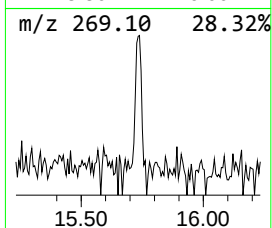
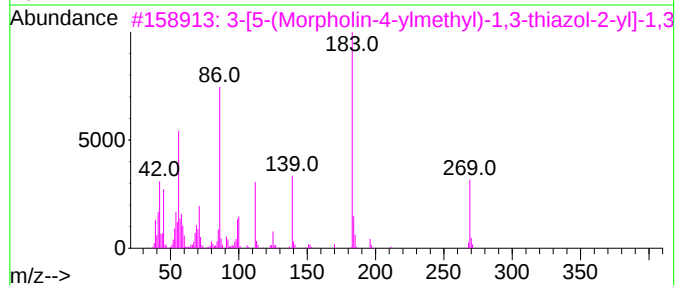
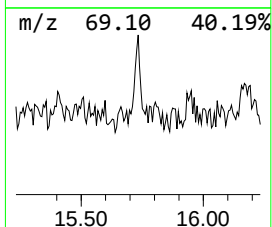
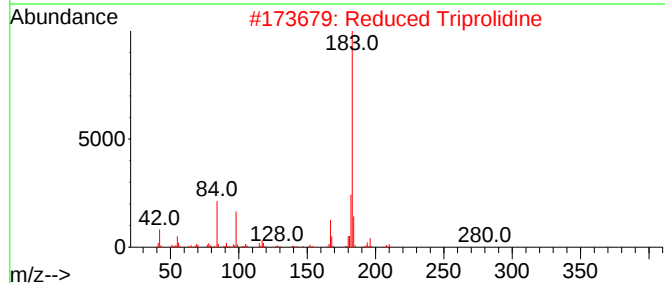
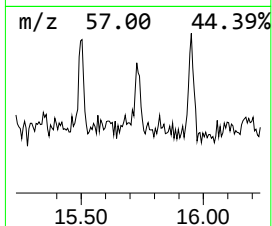
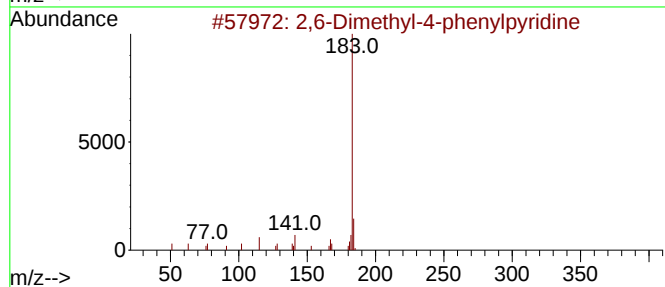
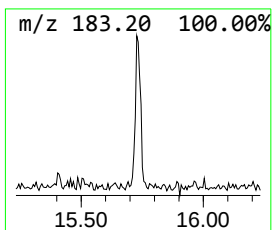
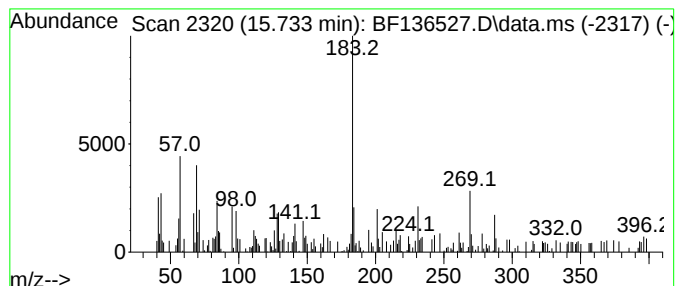
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown15.733 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.733	2.08 ng	55041	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,6-Dimethyl-4-phenylpyridine	183	C13H13N	003044-71-1	38
2			Reduced Triprolidine	280	C19H24N2	1000378-86-2	37
3			3-[5-(Morpholin-4-ylmethyl)-1,3-...	269	C11H15N3O3S	1000410-76-9	32
4			Lauric acid, 3,4-dichlorophenyl ...	344	C18H26Cl2O2	1000357-92-7	32
5			Fumaric acid, 4-chlorophenyl hex...	310	C16H19ClO4	1000344-85-7	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121223\
Data File : BF136527.D
Acq On : 12 Dec 2023 21:03
Operator : CG\JU
Sample : 05470-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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-...	5.034	20.1	ng	514517	1	6.792	511699	20.0
n-Hexadecanoic ...	11.857	4.4	ng	130592	4	11.322	599506	20.0
Adipic acid, 2-...	13.463	10.5	ng	346923	5	13.968	660768	20.0
E-15-Heptadecenal	13.892	3.3	ng	109151	5	13.968	660768	20.0
Benzo[e]pyrene	15.015	2.3	ng	61073	6	15.451	529284	20.0
unknown15.733	15.733	2.1	ng	55041	6	15.451	529284	20.0