

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032124\
 Data File : BF137659.D
 Acq On : 21 Mar 2024 14:16
 Operator : CG\JU
 Sample : PB159682BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB159682BL

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137659.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	483	488	500	rBV	155862	279275	4.12%	0.624%
2	5.351	550	555	558	rBV	5382715	5823351	85.81%	13.017%
3	6.369	723	728	731	rBV	4885897	5927961	87.35%	13.250%
4	6.722	785	788	803	rBV	1413354	1371870	20.22%	3.066%
5	7.292	880	885	888	rBV	3554730	3875277	57.11%	8.662%
6	8.004	1002	1006	1030	rBV	1966712	1846415	27.21%	4.127%
7	9.086	1184	1190	1193	rBV	6863867	6786147	100.00%	15.169%
8	9.757	1300	1304	1320	rBV	2413634	2084180	30.71%	4.659%
9	10.551	1434	1439	1454	rBV	4188421	4037358	59.49%	9.024%
10	11.239	1553	1556	1568	rBV	1996763	2016469	29.71%	4.507%
11	12.651	1793	1796	1800	rBV	201281	174897	2.58%	0.391%
12	12.833	1822	1827	1830	rBV	6836944	6572428	96.85%	14.691%
13	13.357	1913	1916	1921	rBV	151592	136480	2.01%	0.305%
14	13.874	2001	2004	2018	rBV	1359876	1436155	21.16%	3.210%
15	14.651	2132	2136	2142	rBV	105043	104328	1.54%	0.233%
16	14.974	2187	2191	2200	rBV	112140	136243	2.01%	0.305%
17	15.304	2242	2247	2250	rBV	859168	1153216	16.99%	2.578%
18	15.333	2250	2252	2268	rVB	190558	250230	3.69%	0.559%
19	15.745	2317	2322	2332	rVB	117996	176606	2.60%	0.395%
20	16.221	2397	2403	2411	rBV	103366	179777	2.65%	0.402%
21	16.380	2419	2430	2443	rBV4	34122	141428	2.08%	0.316%
22	16.780	2491	2498	2506	rBV2	64211	133275	1.96%	0.298%
23	17.439	2603	2610	2617	rBV2	40331	94585	1.39%	0.211%

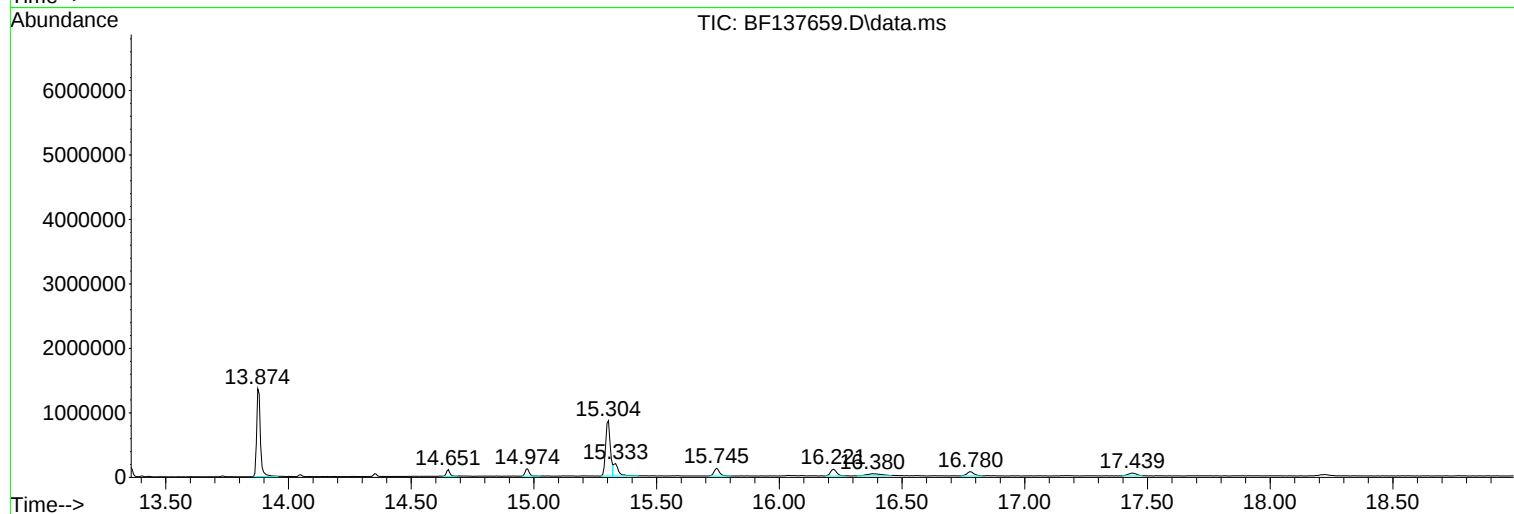
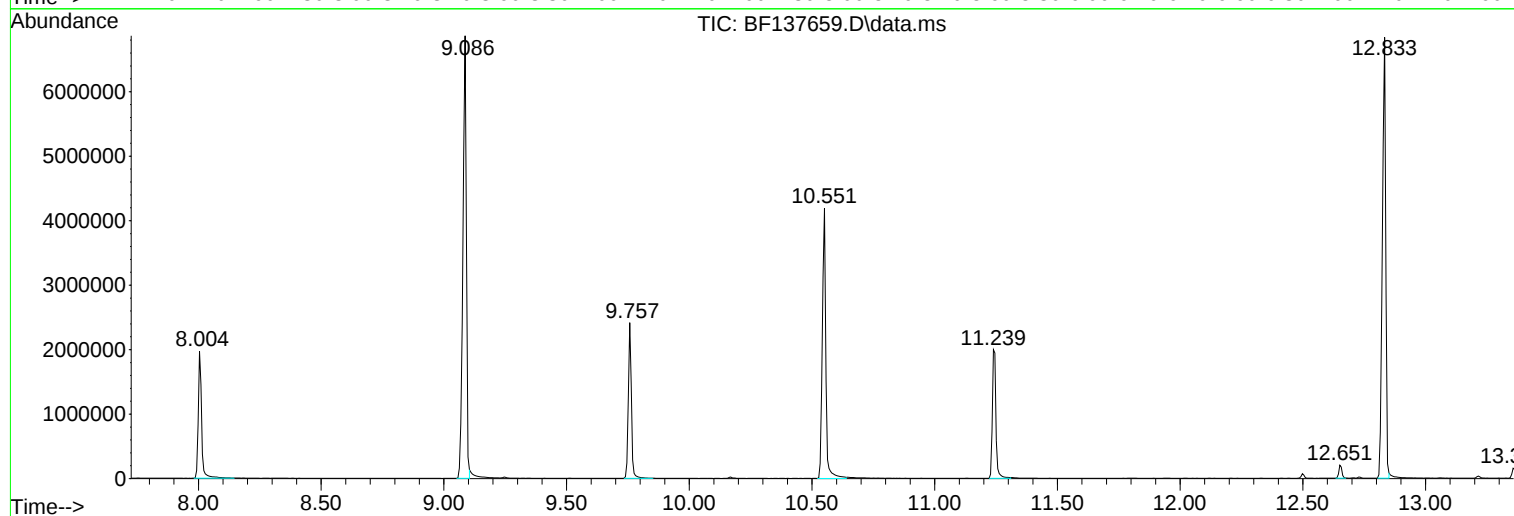
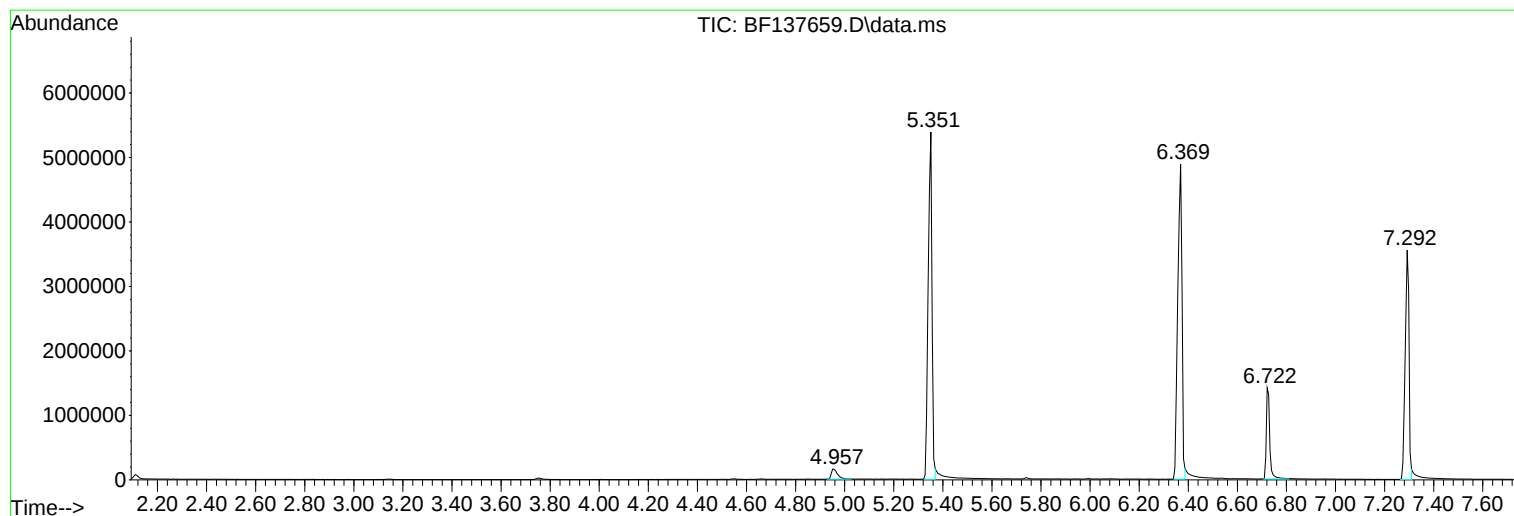
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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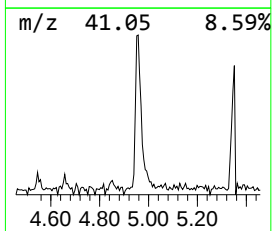
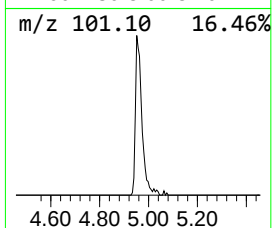
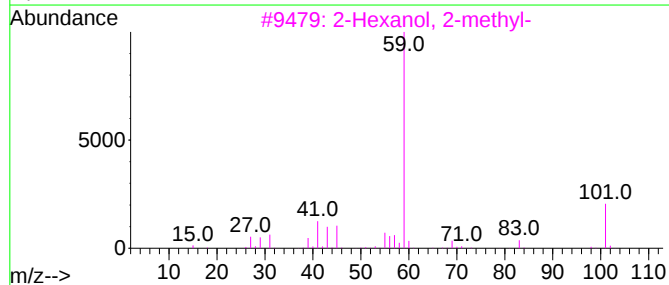
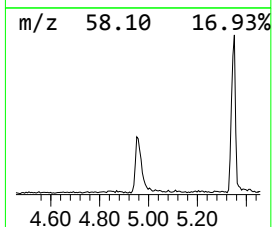
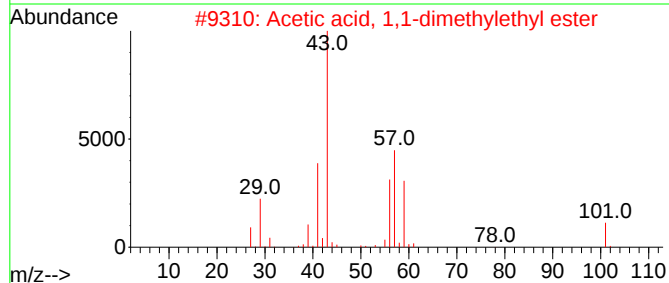
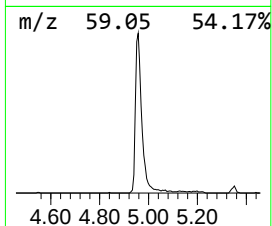
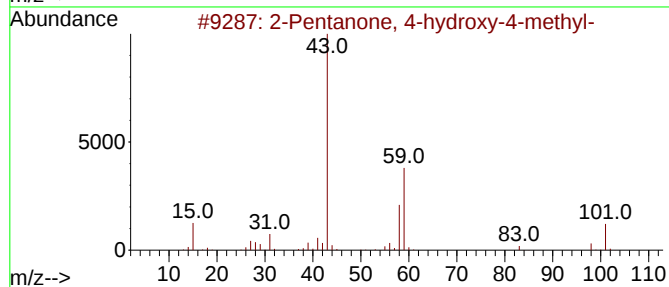
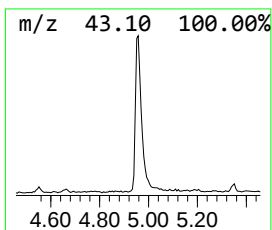
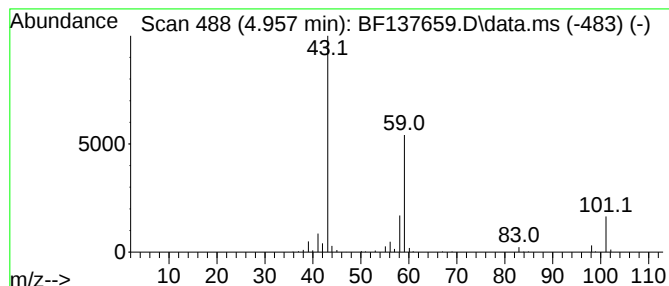
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.957	4.07 ng	279275	1,4-Dichlorobenzene-d4	6.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10		



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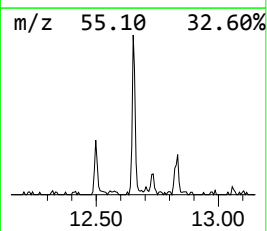
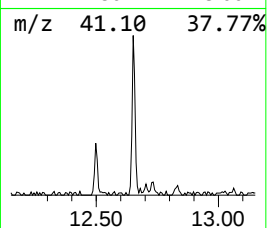
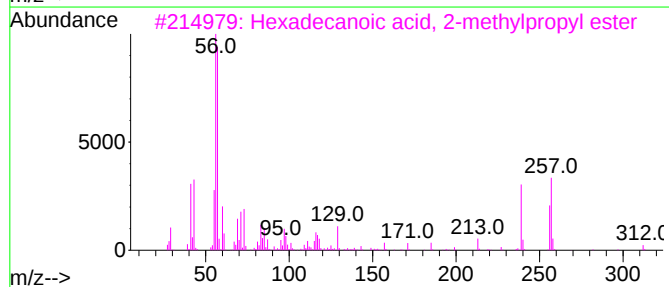
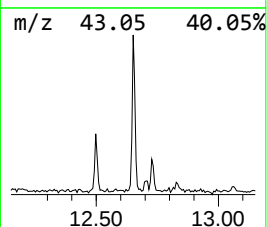
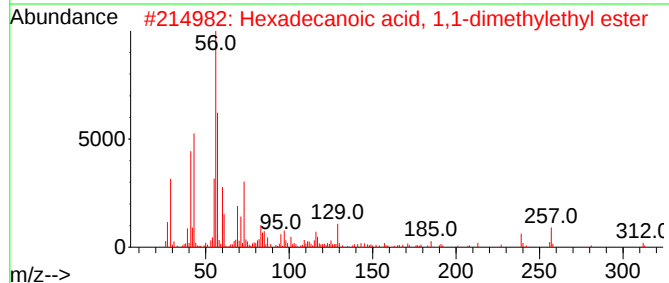
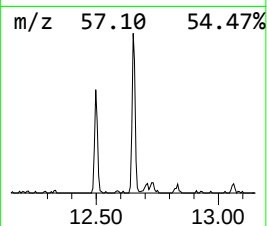
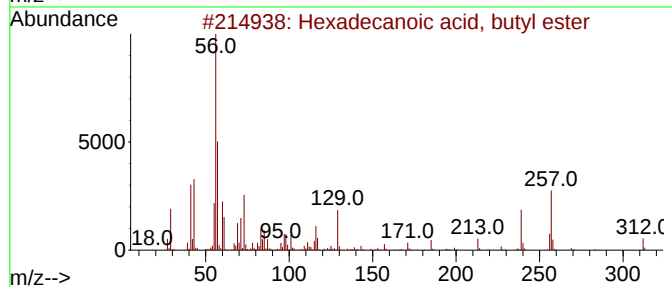
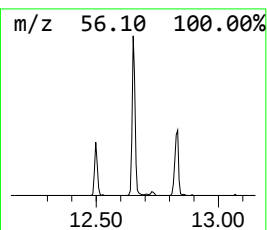
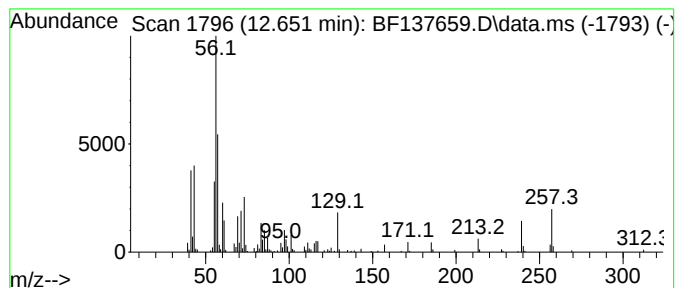
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Peak Number 2 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	2.44 ng	174897	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	43
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	41
4			Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5			1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



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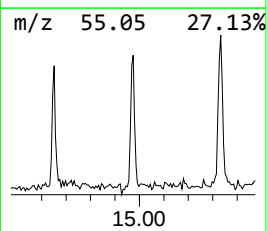
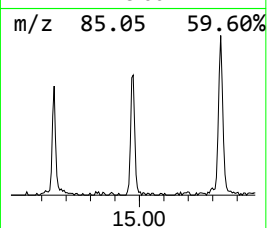
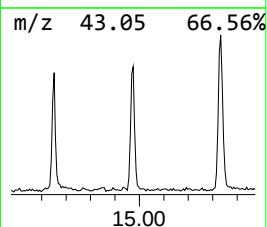
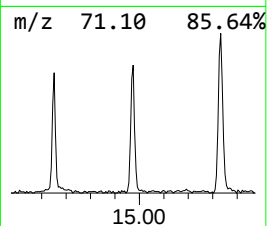
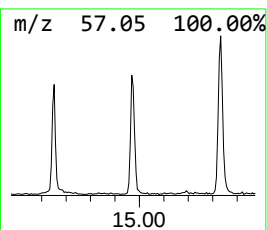
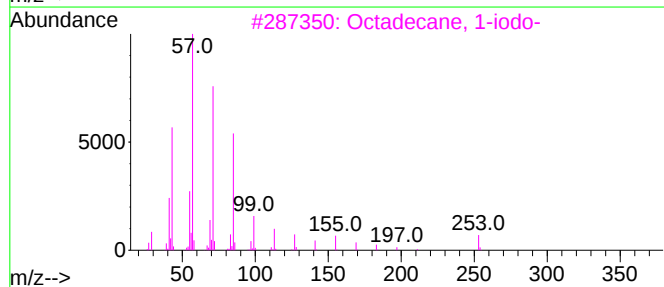
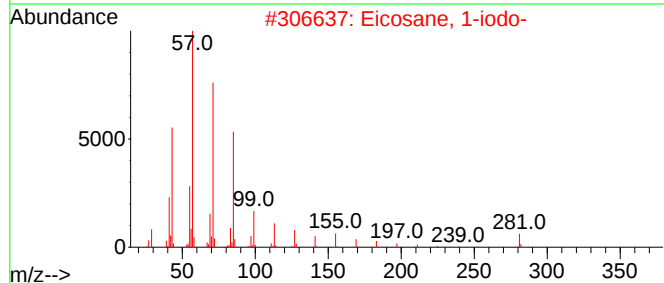
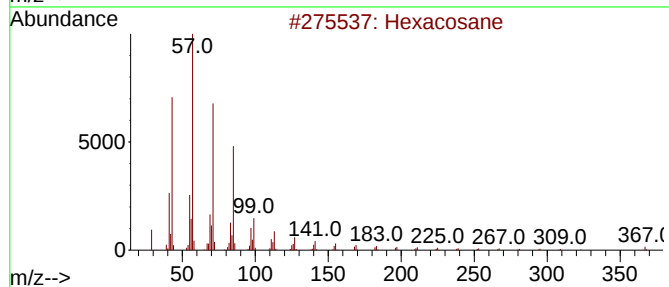
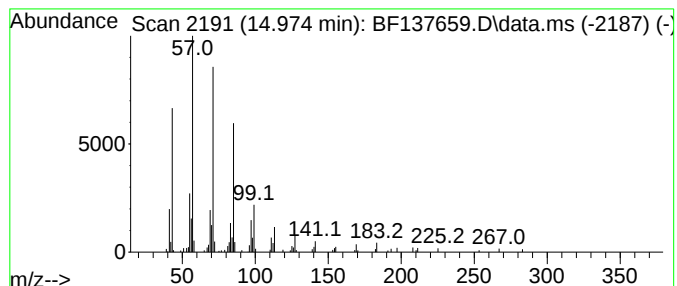
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	2.36 ng	136243	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	91
3			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	91
4			Heneicosane	296	C21H44	000629-94-7	90
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90



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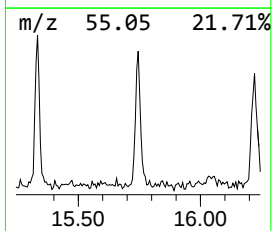
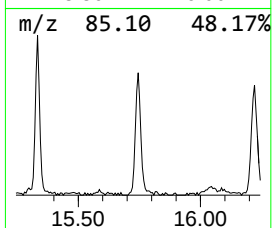
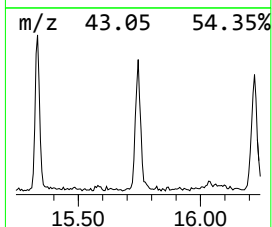
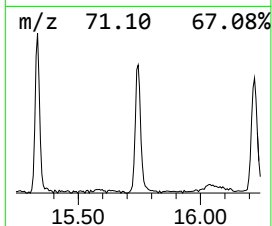
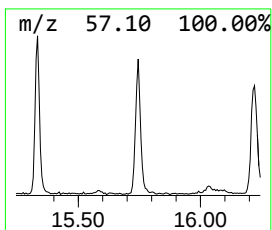
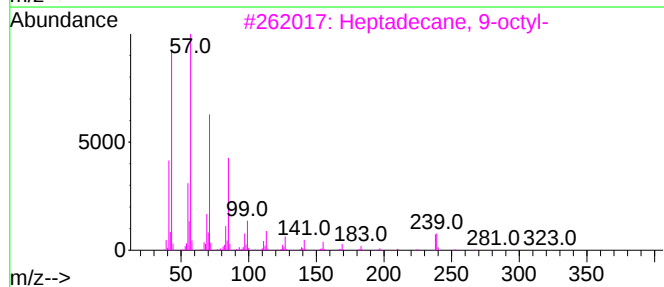
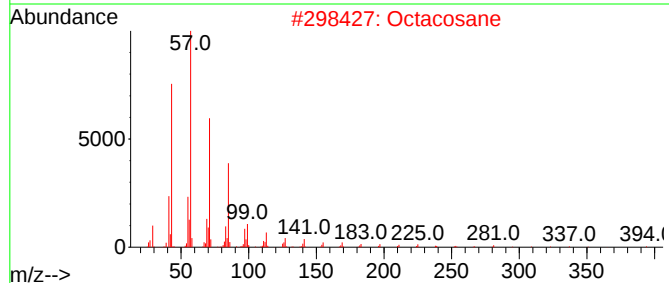
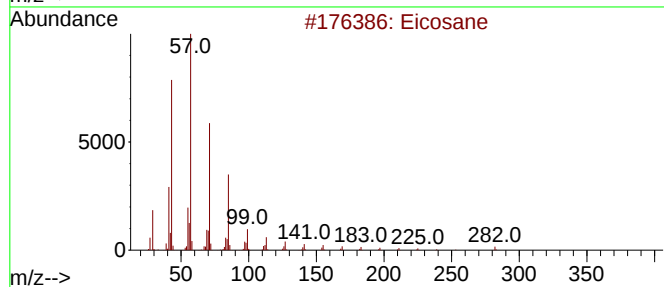
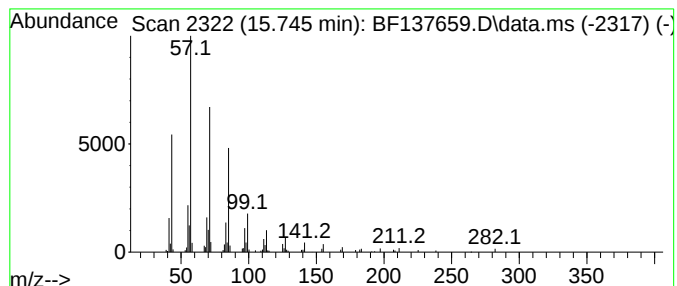
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.745	3.06 ng	176606	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Octacosane	394	C28H58	000630-02-4	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			Heptacosane	380	C27H56	000593-49-7	91
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



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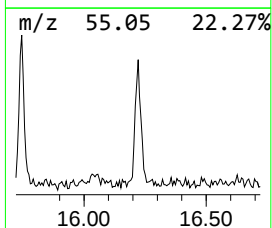
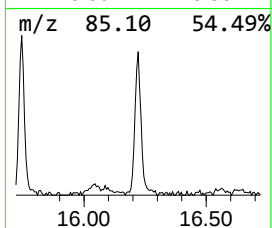
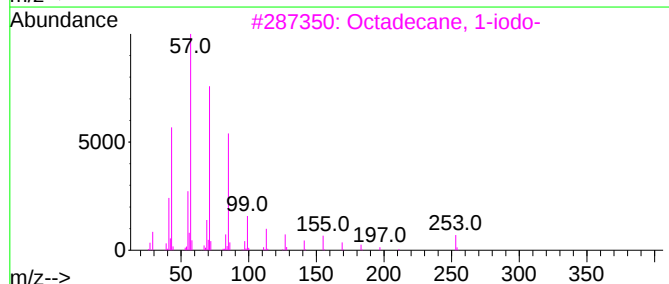
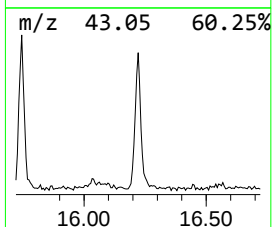
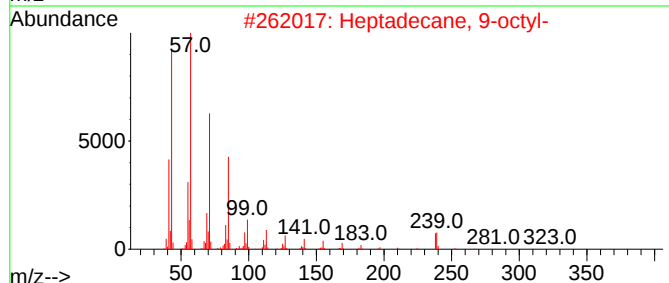
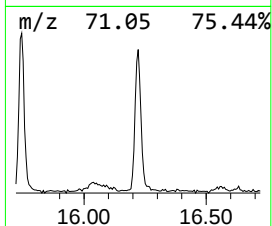
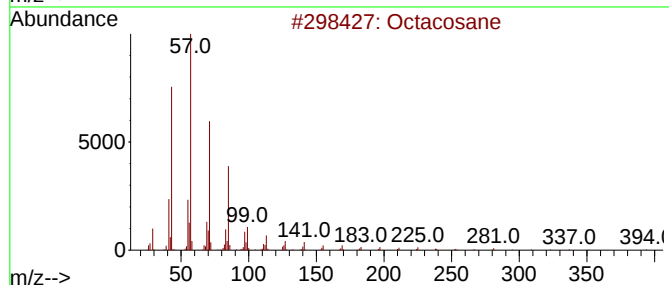
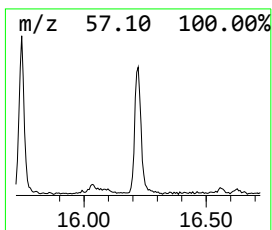
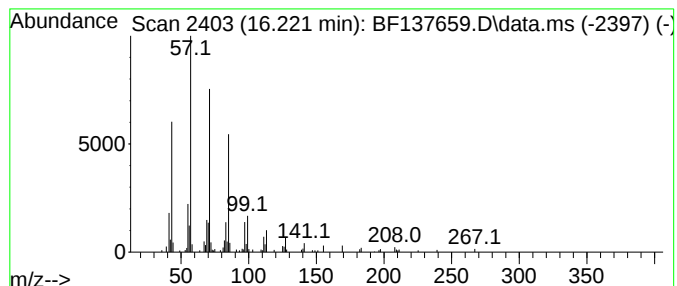
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.221	3.12 ng	179777	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
4			Octadecane	254	C18H38	000593-45-3	87
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86



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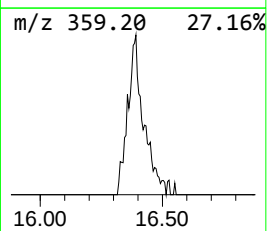
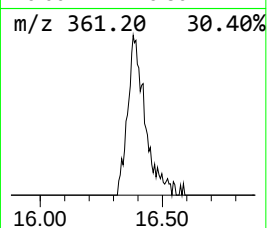
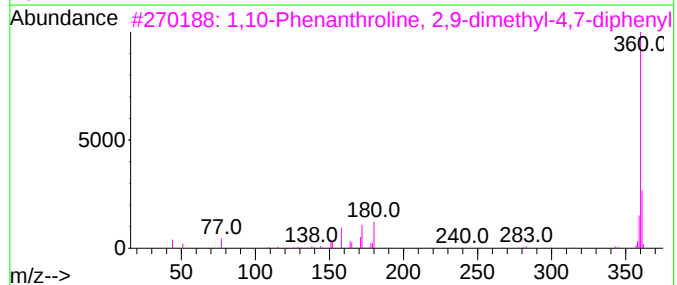
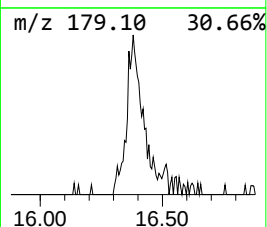
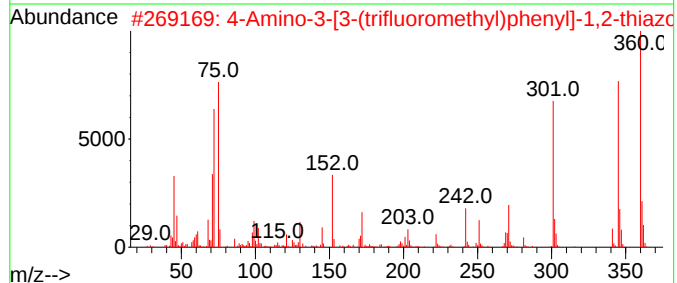
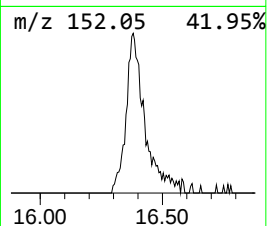
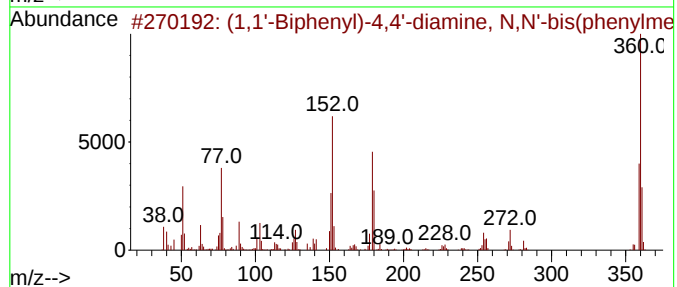
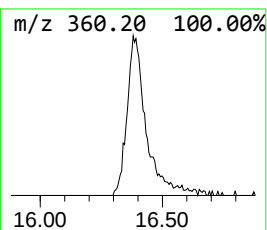
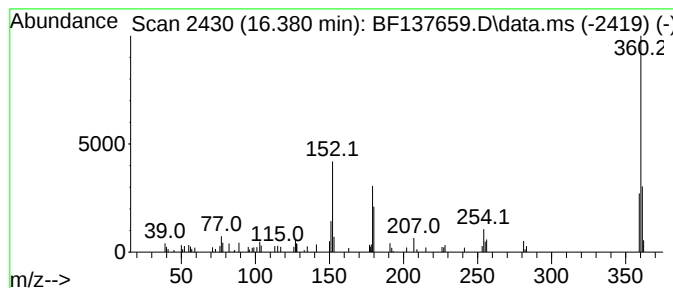
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.380	2.45 ng	141428	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	95
2			4-Amino-3-[3-(trifluoromethyl)ph...	360	C14H15F3N2O2SSi	1010500-98-0	52
3			1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	49
4			Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	47
5			1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032124\
Data File : BF137659.D
Acq On : 21 Mar 2024 14:16
Operator : CG\JU
Sample : PB159682BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB159682BL

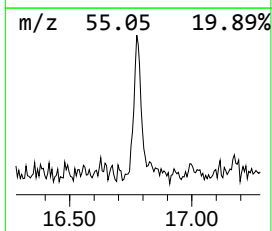
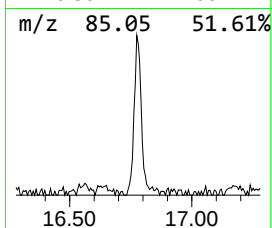
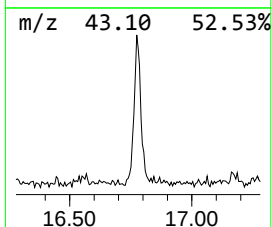
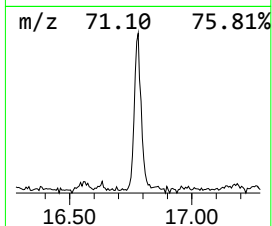
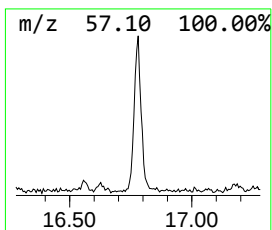
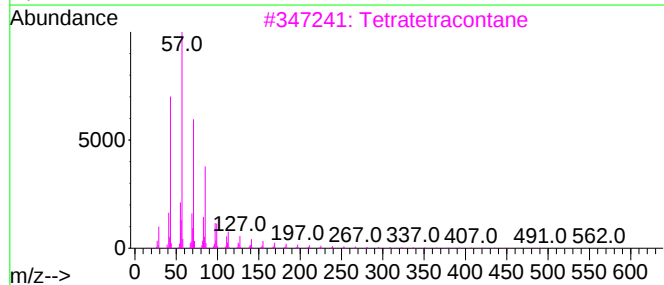
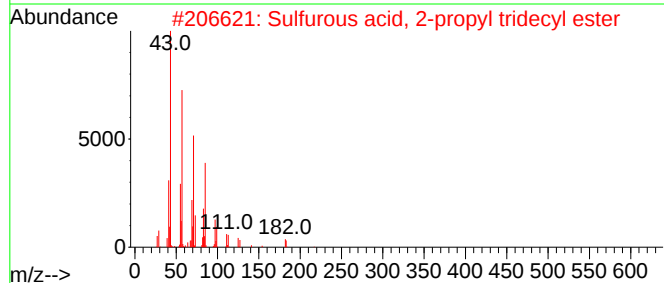
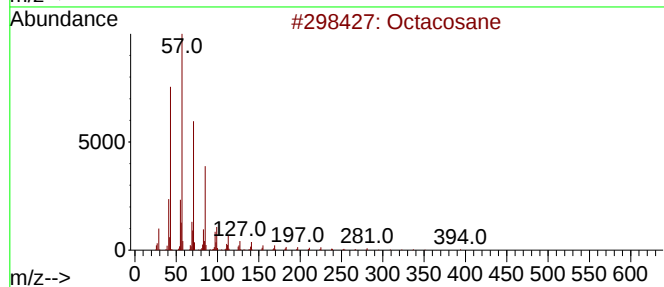
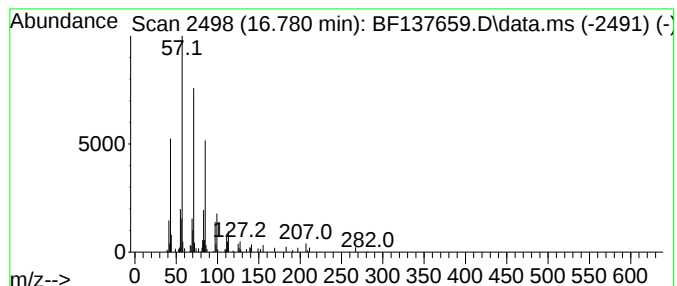
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Sulfurous acid, 2-propyl tr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.780	2.31 ng	133275	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	90
3			Tetratetracontane	619	C44H90	007098-22-8	87
4			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
5			Tetracosane	338	C24H50	000646-31-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032124\
Data File : BF137659.D
Acq On : 21 Mar 2024 14:16
Operator : CG\JU
Sample : PB159682BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB159682BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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
2-Pentanone, 4-...	4.957	4.1	ng	279275	1	6.728	1371870	20.0
Hexadecanoic ac...	12.651	2.4	ng	174897	5	13.874	1436160	20.0
Hexacosane	14.974	2.4	ng	136243	6	15.304	1153220	20.0
Eicosane	15.745	3.1	ng	176606	6	15.304	1153220	20.0
Octacosane	16.221	3.1	ng	179777	6	15.304	1153220	20.0
(1,1'-Biphenyl)...	16.380	2.5	ng	141428	6	15.304	1153220	20.0
Sulfurous acid,...	16.780	2.3	ng	133275	6	15.304	1153220	20.0