

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100224\
 Data File : BF139614.D
 Acq On : 02 Oct 2024 18:46
 Operator : RC/JU
 Sample : P4222-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-5

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-BF100124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139614.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	3	10	17	rVB	1915018	2980569	100.00%	15.499%
2	5.087	498	509	517	rBV	108906	180481	6.06%	0.939%
3	5.487	570	577	582	rBV	1720187	2299064	77.14%	11.956%
4	6.499	742	749	754	rBV	1723146	2407225	80.76%	12.518%
5	6.863	806	811	816	rBV	394348	486183	16.31%	2.528%
6	7.428	901	907	912	rBV	1196029	1555105	52.17%	8.087%
7	8.145	1024	1029	1042	rVB	497446	617433	20.72%	3.211%
8	9.222	1206	1212	1217	rBV	2072839	2536255	85.09%	13.189%
9	9.898	1322	1327	1332	rBV	504897	624262	20.94%	3.246%
10	10.616	1443	1449	1456	rBV	226512	281610	9.45%	1.464%
11	10.686	1456	1461	1477	rBV	998058	1330131	44.63%	6.917%
12	11.386	1575	1580	1588	rBV	447474	551042	18.49%	2.866%
13	11.910	1662	1669	1681	rBV	223824	359583	12.06%	1.870%
14	12.439	1755	1759	1771	rVB3	12659	29956	1.01%	0.156%
15	12.598	1782	1786	1790	rBV	28946	40495	1.36%	0.211%
16	12.698	1798	1803	1814	rBV	40556	73602	2.47%	0.383%
17	12.975	1844	1850	1855	rBV	1322081	1696802	56.93%	8.824%
18	13.875	1998	2003	2018	rBV	73559	146630	4.92%	0.762%
19	14.027	2021	2029	2039	rVV	350733	503091	16.88%	2.616%
20	14.492	2104	2108	2113	rBV	21652	34853	1.17%	0.181%
21	14.874	2169	2173	2181	rVB	29674	44229	1.48%	0.230%
22	15.069	2202	2206	2213	rBV	15021	36296	1.22%	0.189%
23	15.498	2273	2279	2291	rVB	245120	415271	13.93%	2.159%

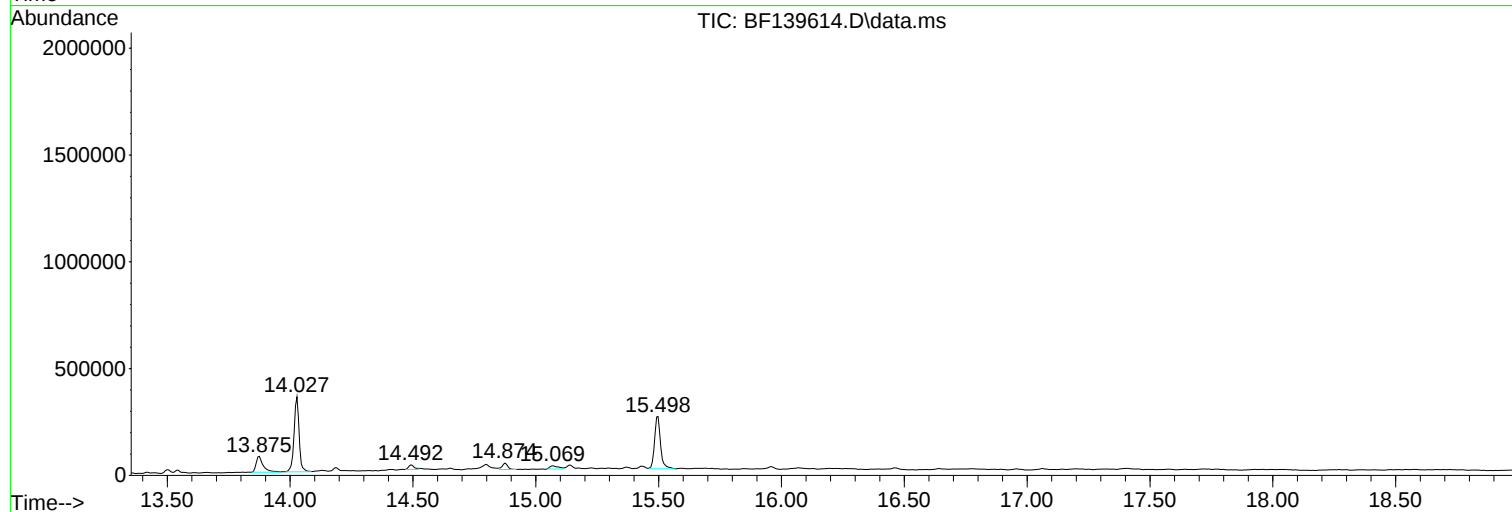
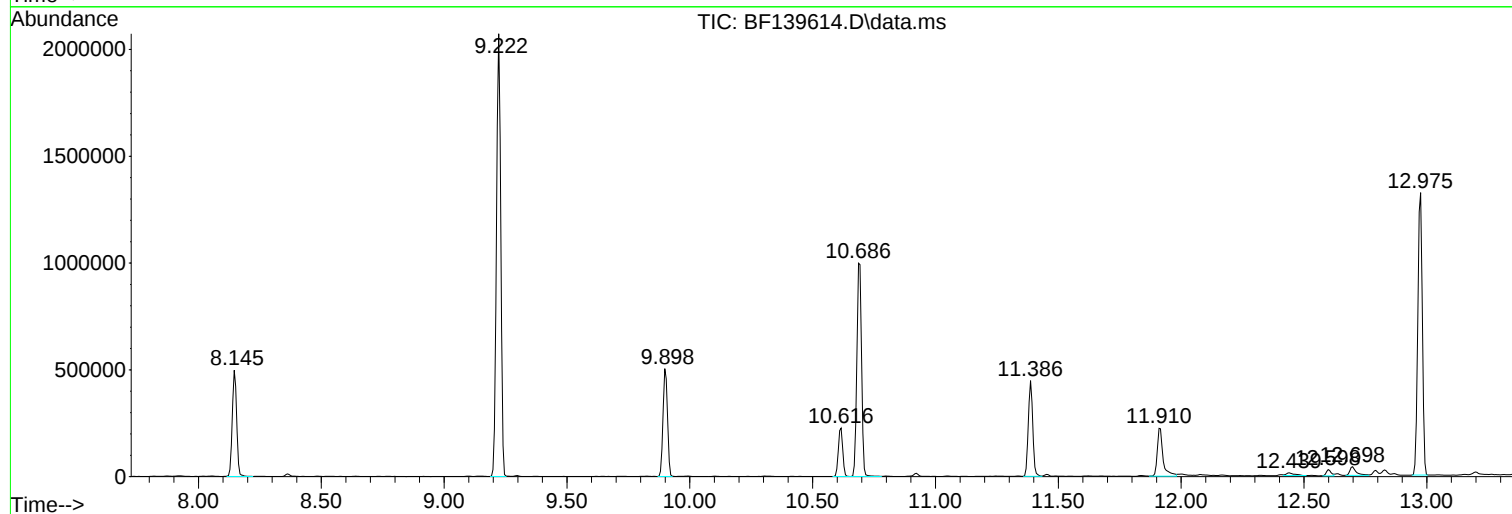
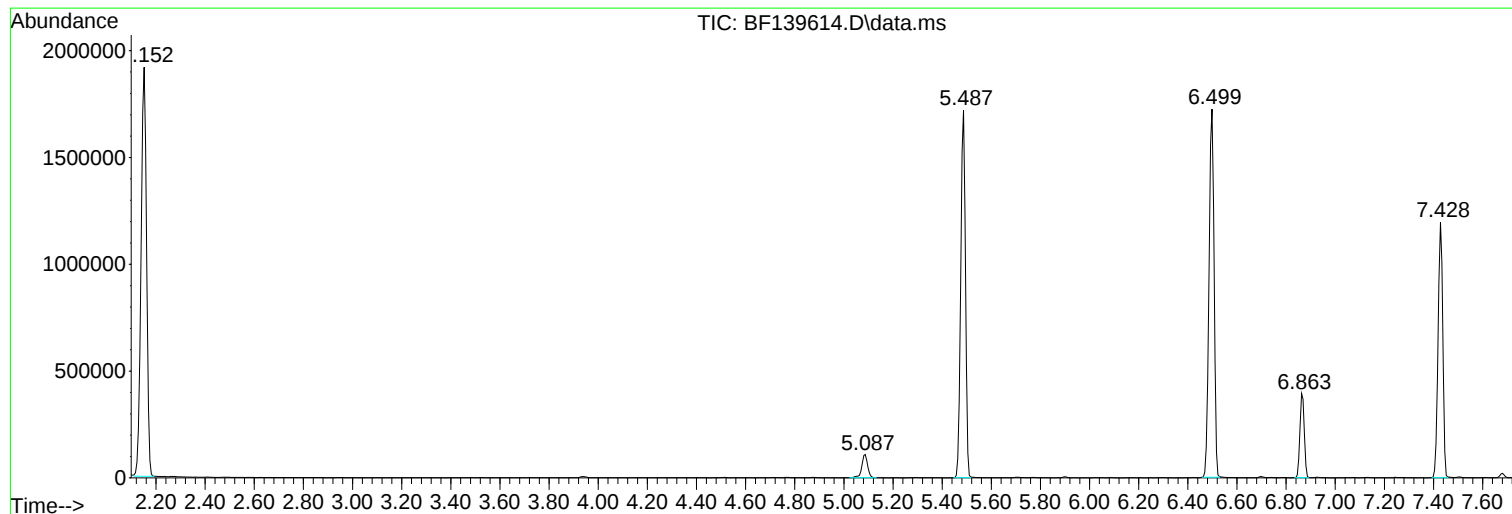
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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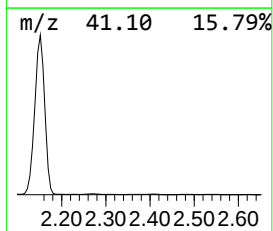
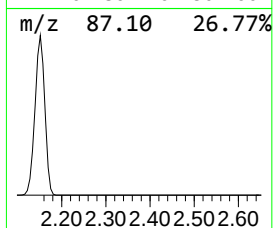
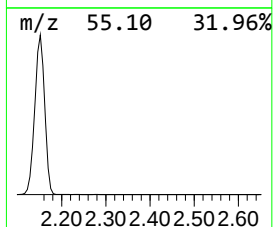
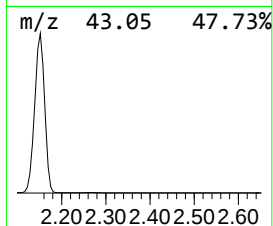
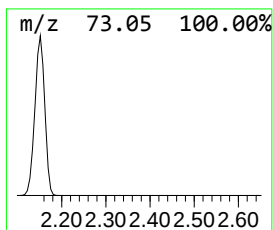
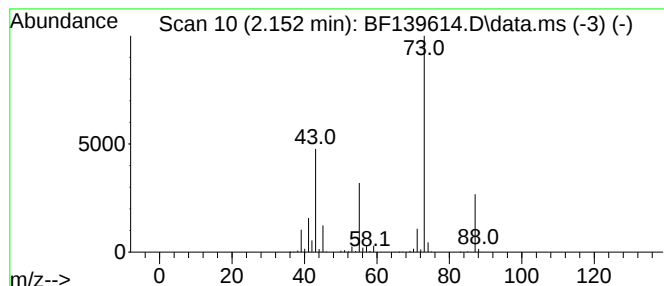
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	122.61 ng	2980570	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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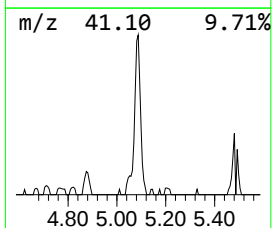
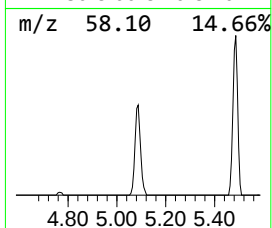
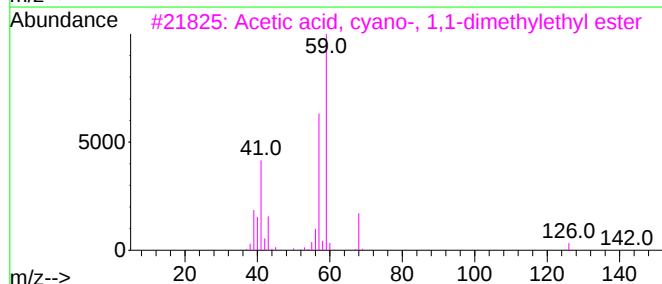
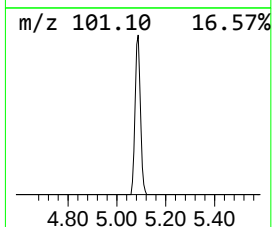
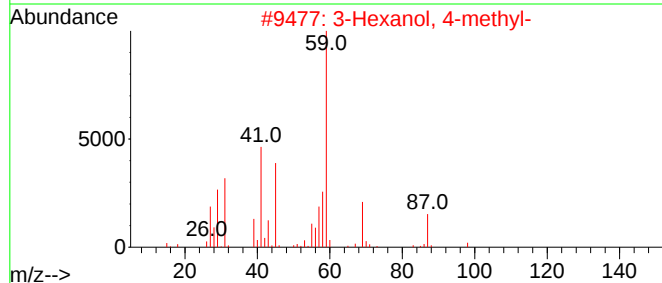
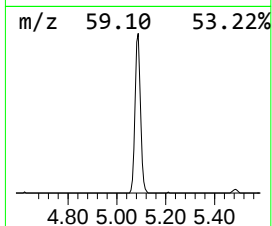
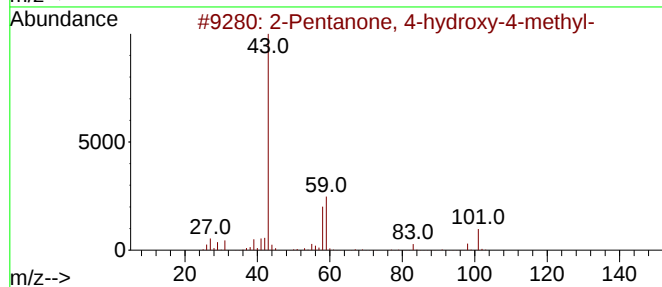
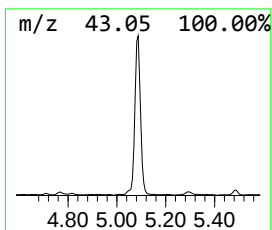
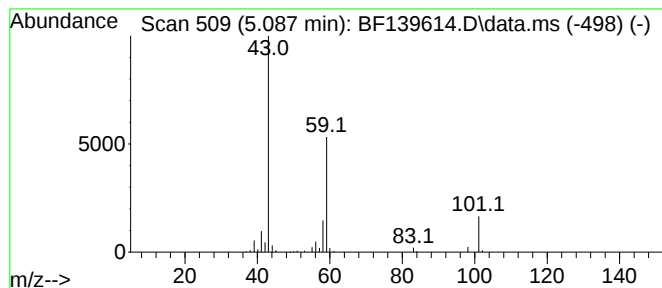
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	7.42 ng	180481	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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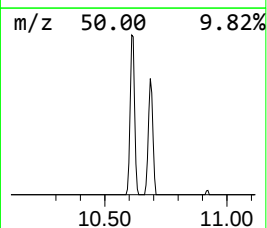
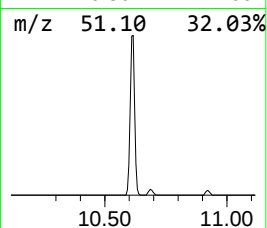
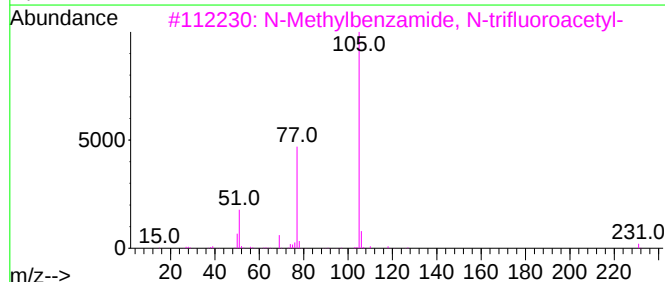
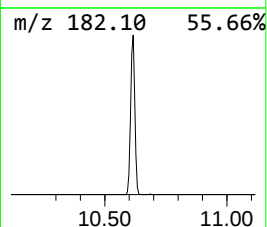
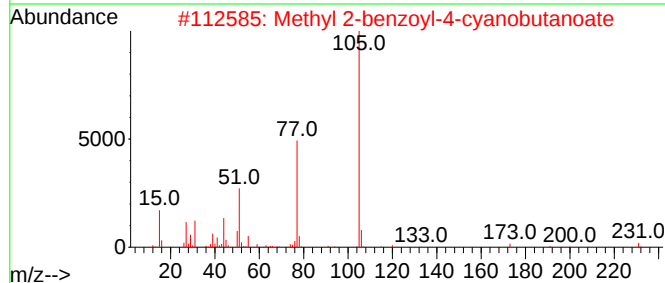
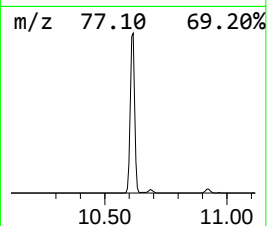
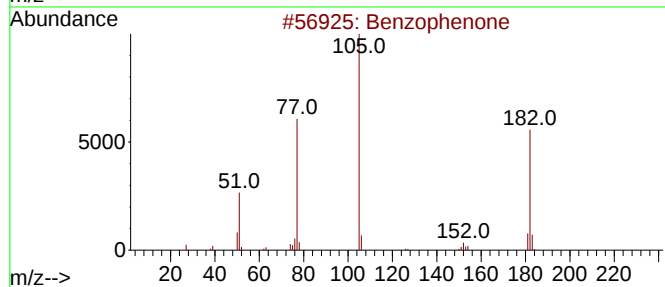
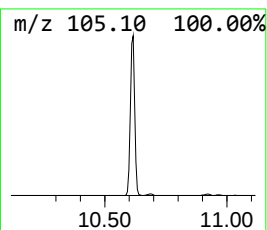
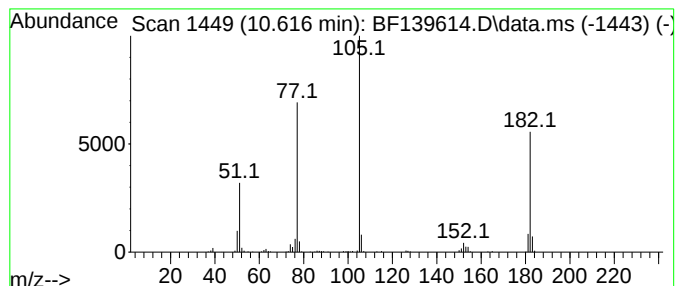
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Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.616	9.02 ng	281610	Acenaphthene-d10	9.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	50
3			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	50
4			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	50
5			N-Methylbenzamide, N-heptafluoro...	331	C12H8F7NO2	1000446-97-2	50



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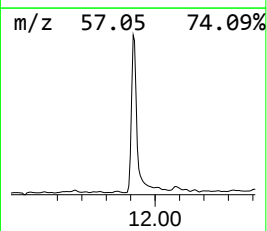
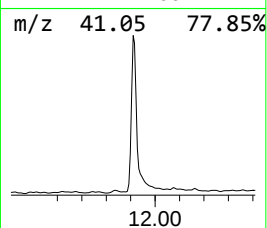
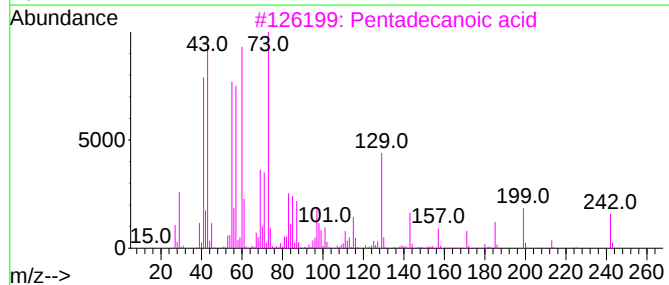
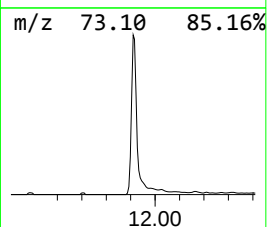
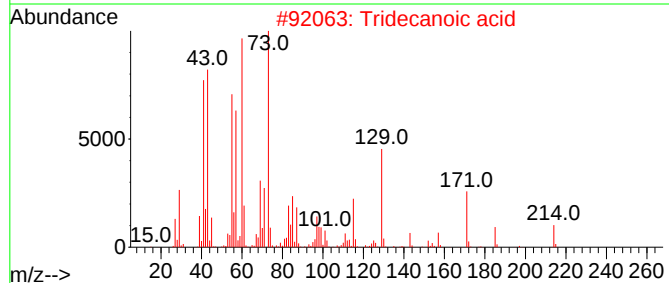
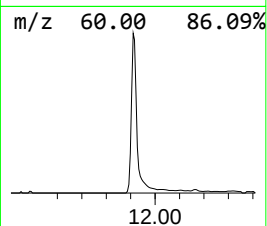
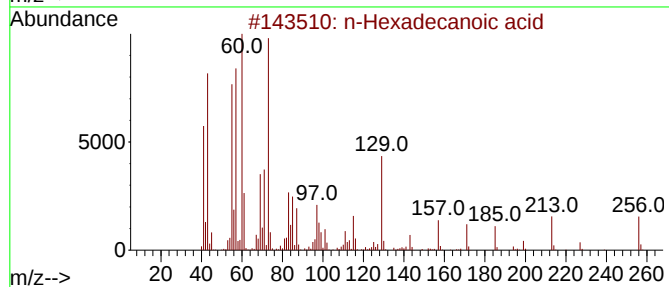
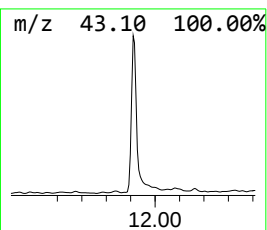
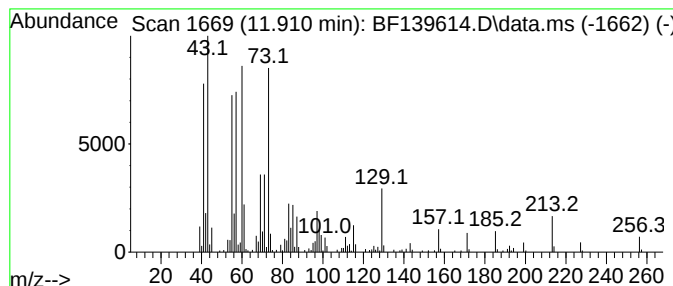
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	13.05 ng	359583	Phenanthrene-d10	11.386

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	58



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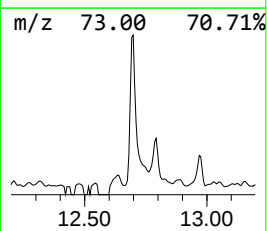
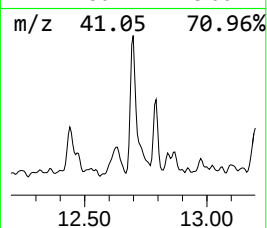
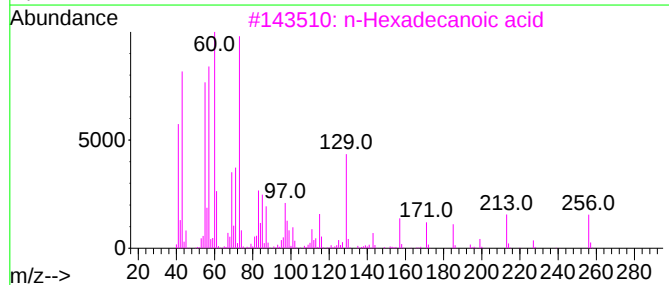
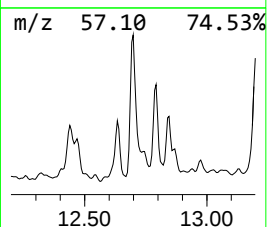
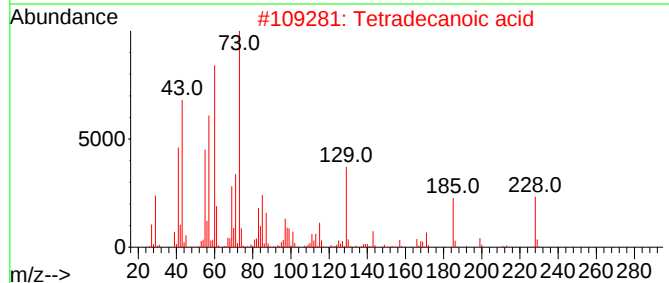
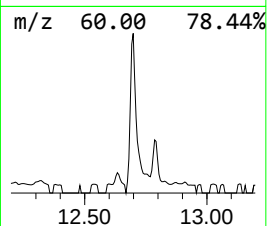
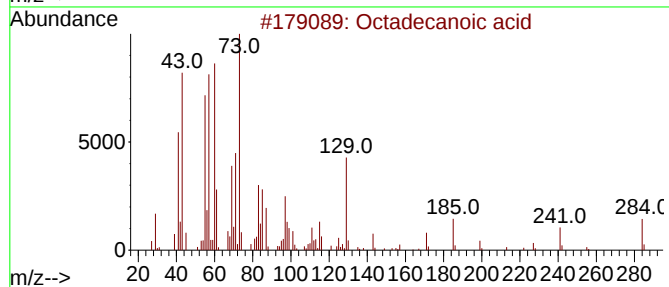
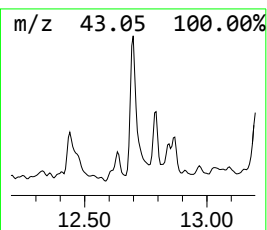
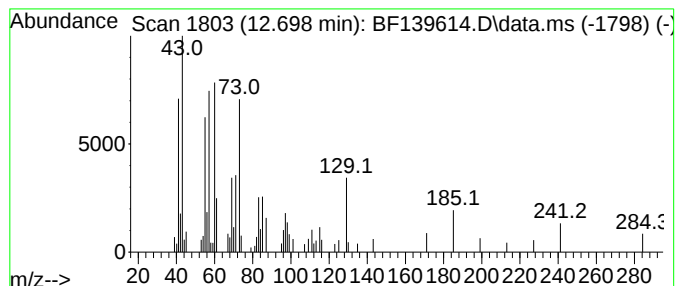
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.698	2.67 ng	73602	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
4			n-Decanoic acid	172	C10H20O2	000334-48-5	43
5			11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	43



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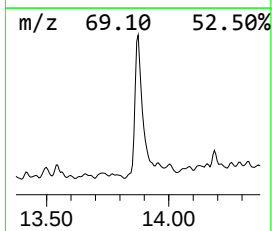
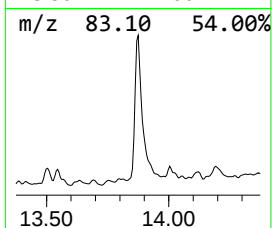
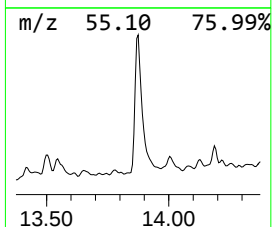
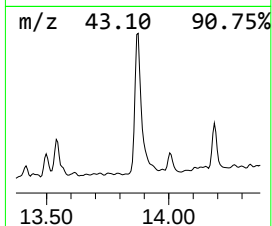
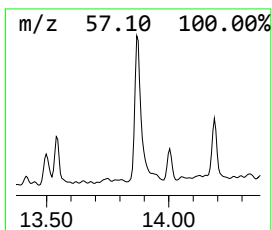
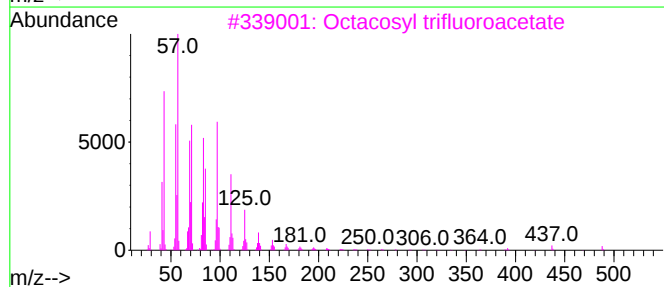
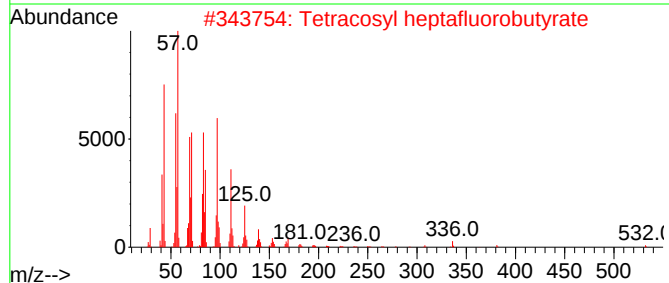
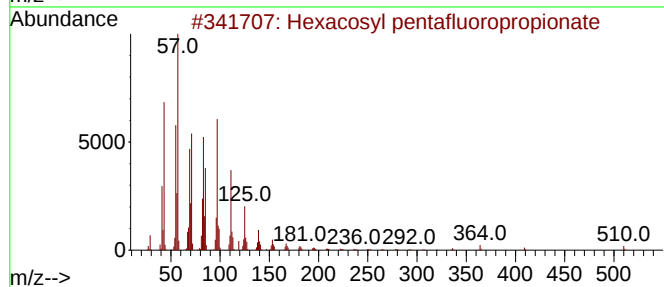
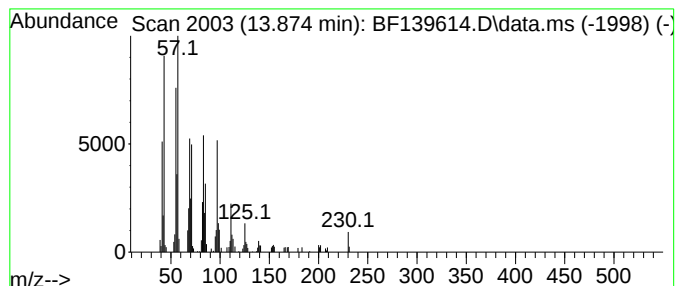
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosyl pentafluoropropio... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	5.83 ng	146630	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91
2			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
3			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
4			Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	91
5			Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100224\
Data File : BF139614.D
Acq On : 02 Oct 2024 18:46
Operator : RC/JU
Sample : P4222-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

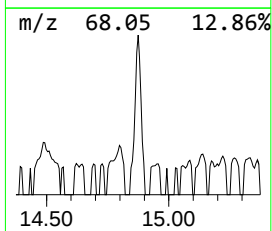
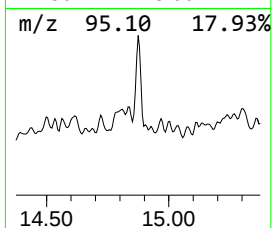
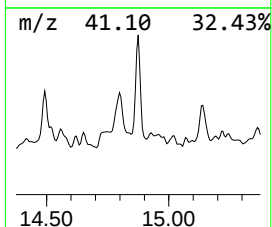
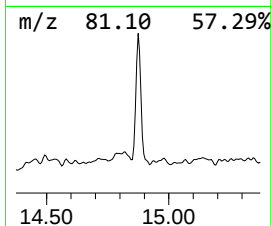
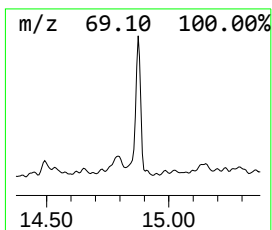
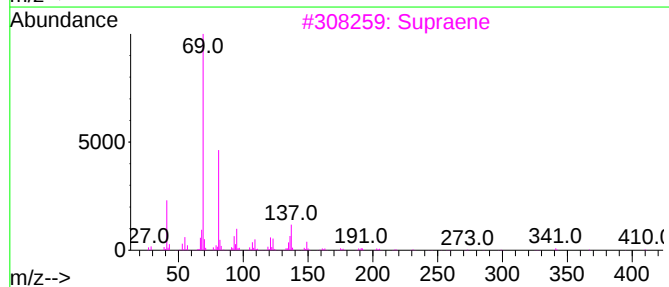
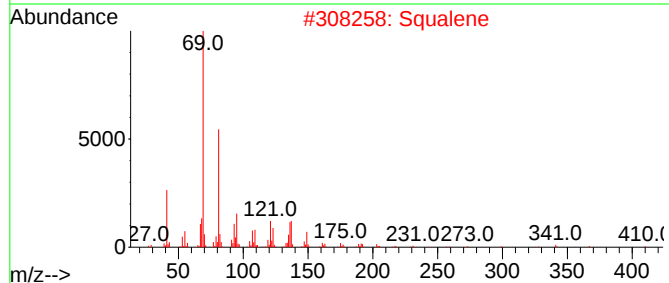
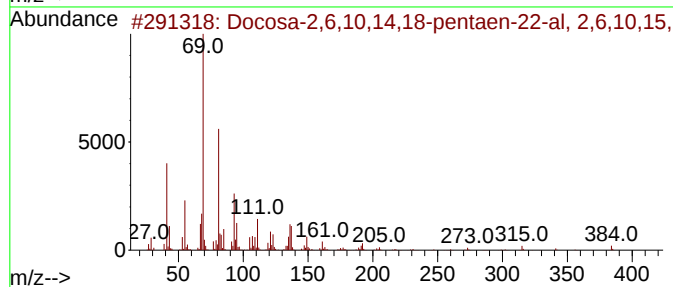
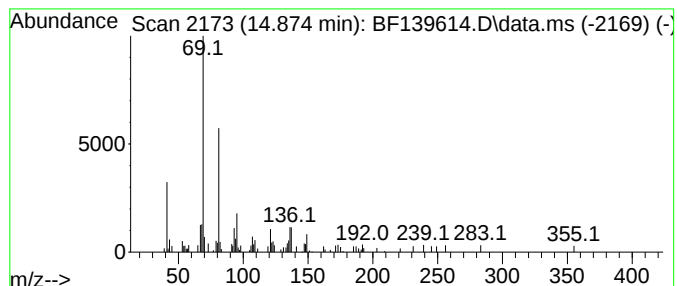
Instrument :
BNA_F
ClientSampleId :
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Docosa-2,6,10,14,18-pentaen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.874	2.13 ng	44229	Perylene-d12	15.498	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	91
2	Squalene	410	C30H50	000111-02-4	87
3	Supraene	410	C30H50	007683-64-9	86
4	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	74
5	trans-Farnesol	222	C15H26O	000106-28-5	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100224\
Data File : BF139614.D
Acq On : 02 Oct 2024 18:46
Operator : RC/JU
Sample : P4222-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF100124.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
Butane, 2-metho...	2.152	122.6	ng	2980570	1	6.863	486183	20.0
2-Pentanone, 4-...	5.087	7.4	ng	180481	1	6.863	486183	20.0
Benzophenone	10.616	9.0	ng	281610	3	9.898	624262	20.0
n-Hexadecanoic ...	11.910	13.1	ng	359583	4	11.386	551042	20.0
Octadecanoic acid	12.698	2.7	ng	73602	4	11.386	551042	20.0
Hexacosyl penta...	13.874	5.8	ng	146630	5	14.027	503091	20.0
Docosa-2,6,10,1...	14.874	2.1	ng	44229	6	15.498	415271	20.0