

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051023\
 Data File : BF133330.D
 Acq On : 10 May 2023 14:55
 Operator : CG\JU
 Sample : 02719-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-04_0-2_20230509

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: BF133330.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.263	365	370	376	rBV	88029	109872	2.06%	0.285%
2	4.916	476	481	497	rVB	1391473	1834548	34.48%	4.756%
3	5.340	549	553	557	rBV	4525895	4800845	90.22%	12.447%
4	5.728	616	619	628	rBV	179635	154063	2.90%	0.399%
5	6.369	723	728	731	rBV	4593006	4823374	90.64%	12.505%
6	6.722	784	788	791	rBV	1639283	1242130	23.34%	3.220%
7	7.287	880	884	887	rBV	3192756	3201438	60.16%	8.300%
8	8.004	1003	1006	1010	rBV	2153777	1728427	32.48%	4.481%
9	9.086	1185	1190	1193	rBV	5929380	5321327	100.00%	13.796%
10	9.757	1300	1304	1308	rBV	2460957	1966214	36.95%	5.098%
11	10.469	1421	1425	1429	rBV	349492	272287	5.12%	0.706%
12	10.545	1434	1438	1451	rBV	2441179	2152506	40.45%	5.581%
13	11.239	1552	1556	1559	rBV	2321890	1965497	36.94%	5.096%
14	11.263	1559	1560	1563	rVB	163384	93243	1.75%	0.242%
15	11.774	1642	1647	1658	rBV2	231302	388548	7.30%	1.007%
16	12.039	1687	1692	1700	rVB2	113275	169006	3.18%	0.438%
17	12.451	1759	1762	1765	rVB	122315	99575	1.87%	0.258%
18	12.557	1775	1780	1793	rBV3	189028	437909	8.23%	1.135%
19	12.680	1798	1801	1803	rVB	86573	84040	1.58%	0.218%
20	12.827	1822	1826	1830	rBV	4780352	4841844	90.99%	12.553%
21	13.751	1978	1983	1992	rBV3	146946	374685	7.04%	0.971%
22	13.874	2000	2004	2008	rBV	1287664	1176812	22.12%	3.051%
23	14.051	2032	2034	2039	rVB3	59767	56817	1.07%	0.147%
24	14.357	2084	2086	2089	rVB	71975	60275	1.13%	0.156%
25	15.298	2242	2246	2250	rBV	1090893	1215804	22.85%	3.152%

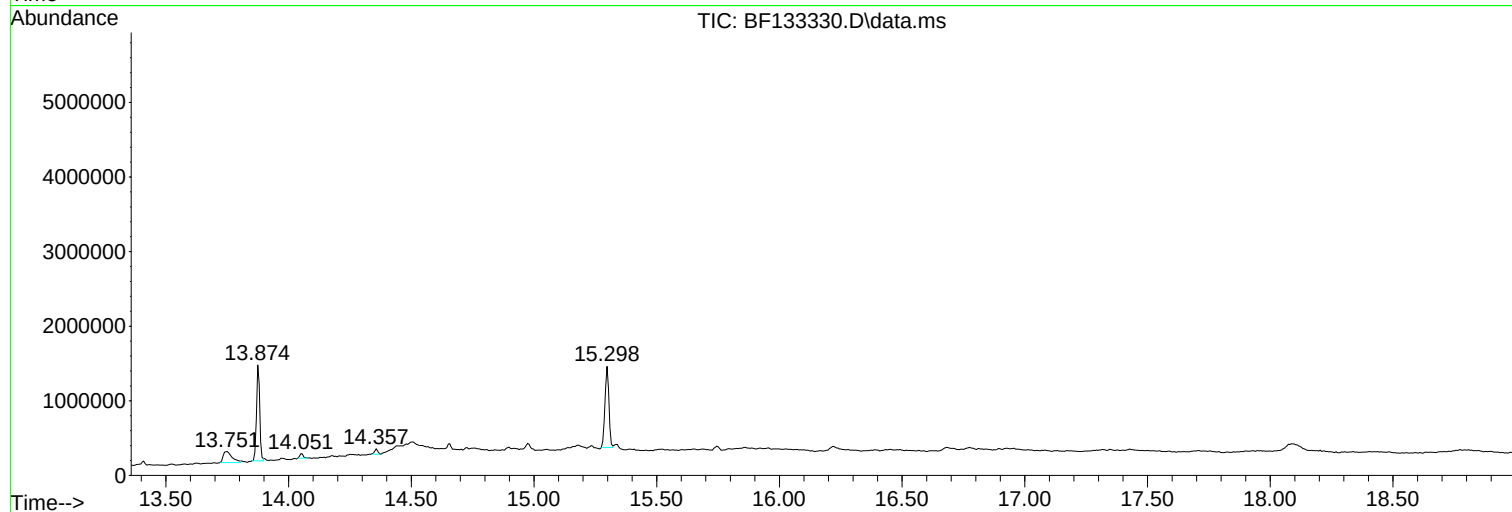
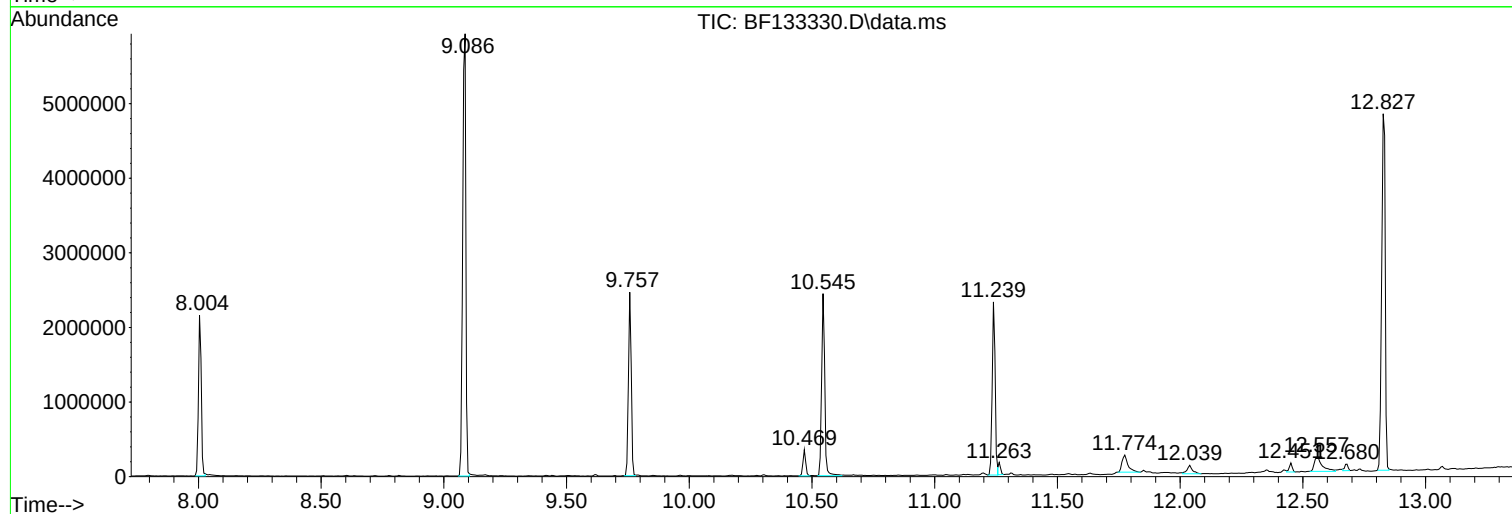
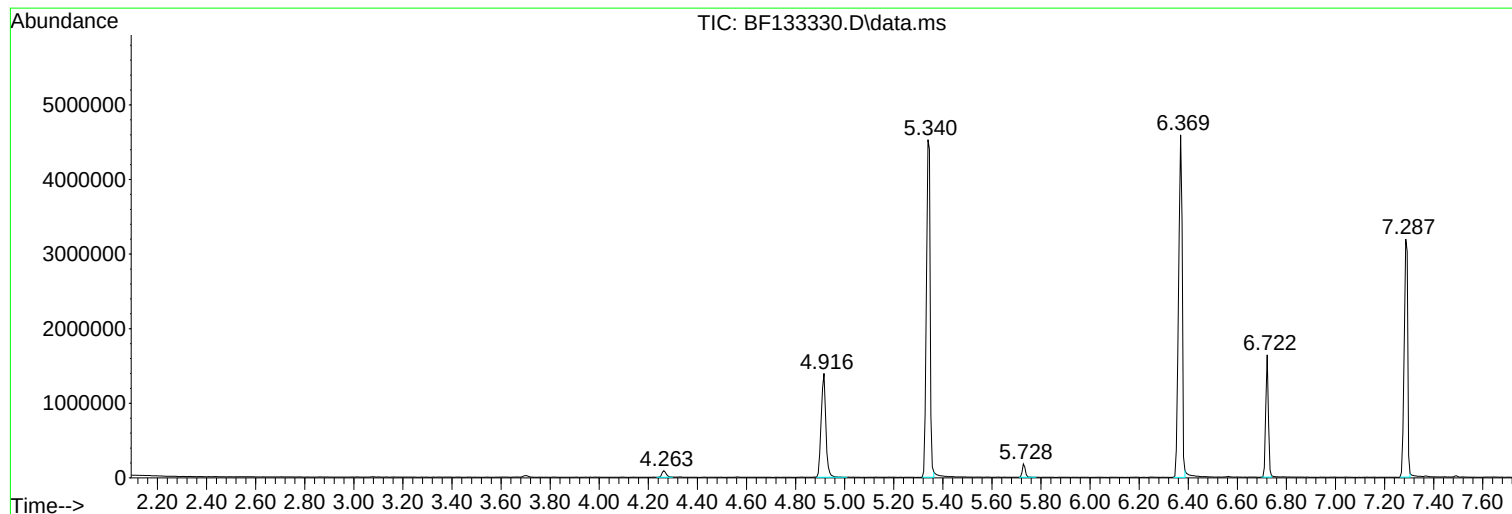
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ClientSampleId :
SB-04_0-2_20230509

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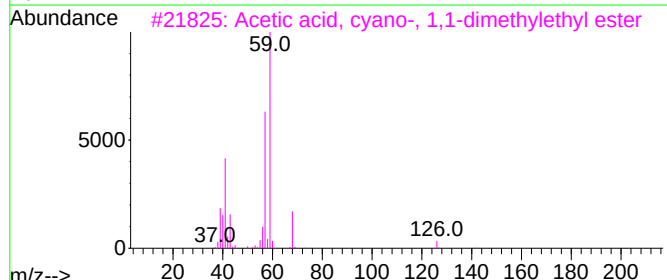
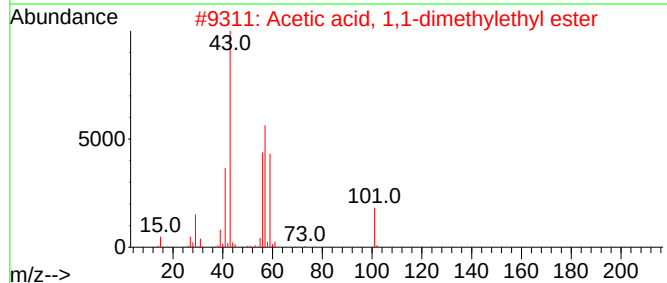
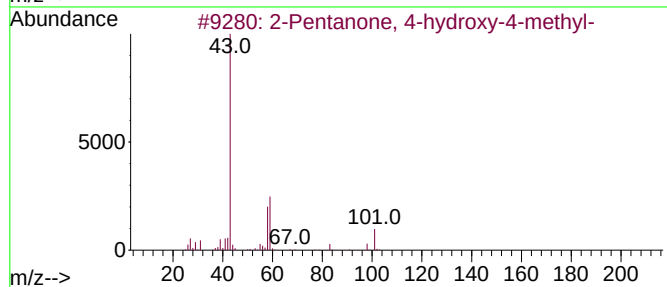
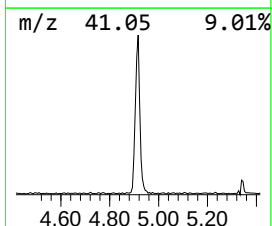
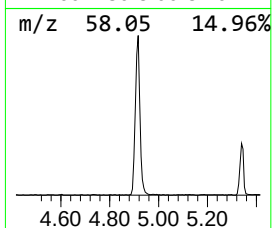
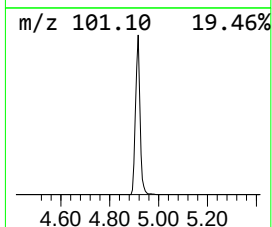
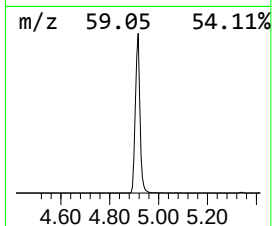
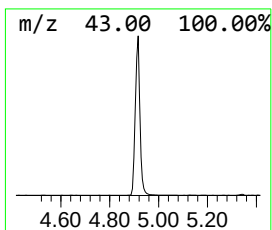
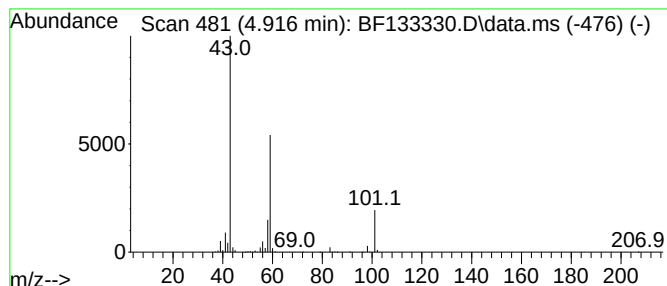
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.916	29.54 ng	1834550	1,4-Dichlorobenzene-d4	6.722	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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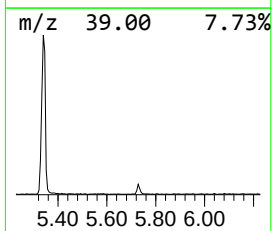
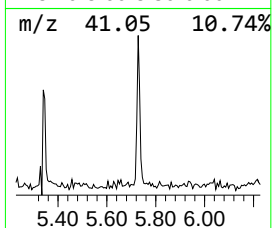
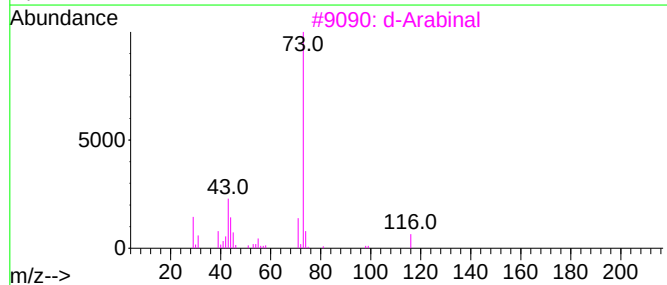
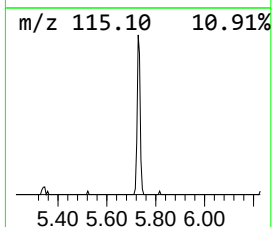
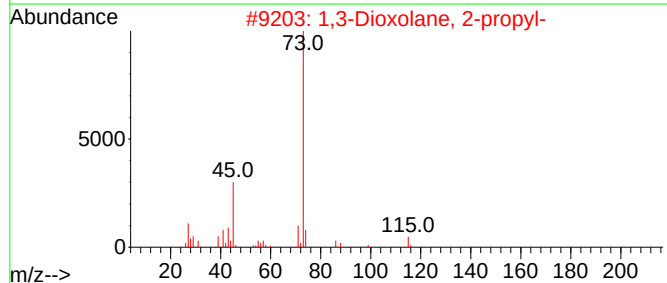
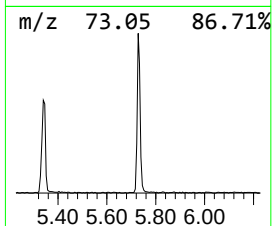
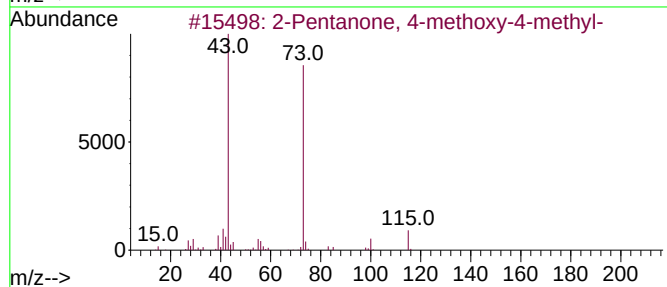
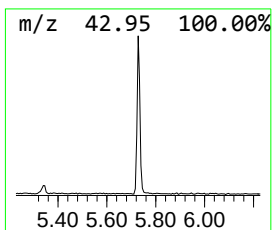
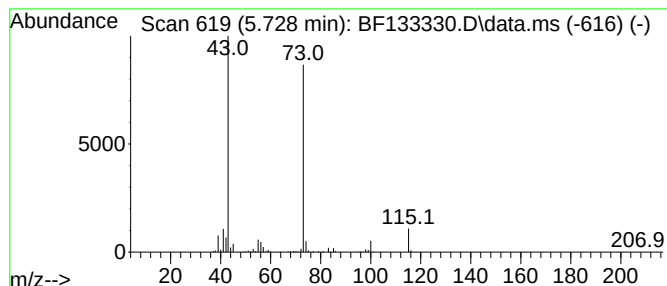
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.728	2.48 ng	154063	1,4-Dichlorobenzene-d4	6.722	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	12
3	d-Arabinol	116	C5H8O3	000496-61-7	12
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	12
5	3-Methoxy-3-methylbutanol	118	C6H14O2	056539-66-3	12



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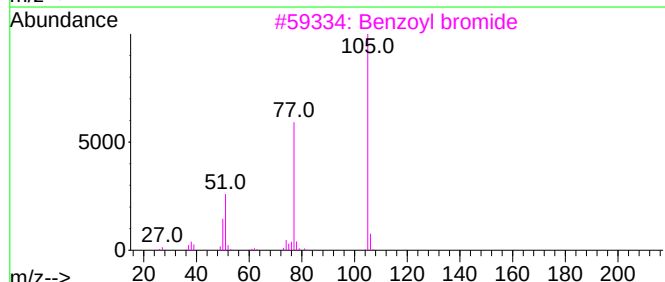
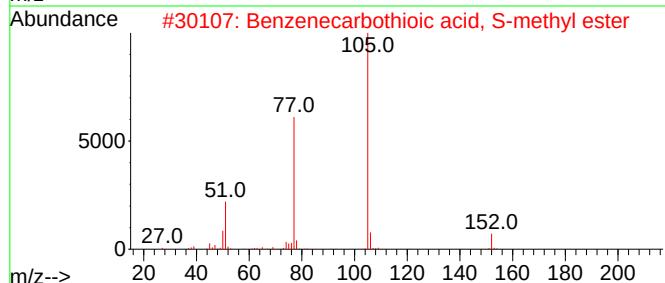
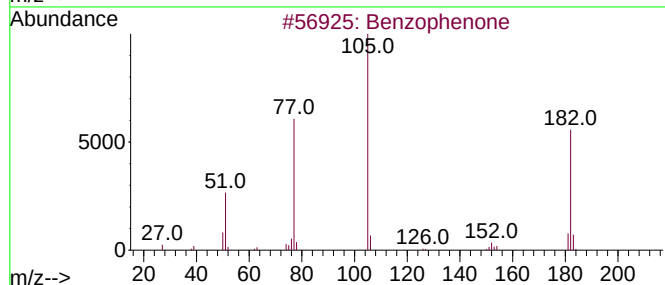
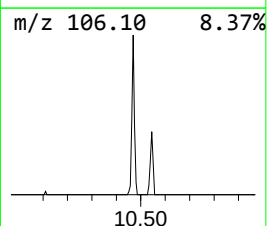
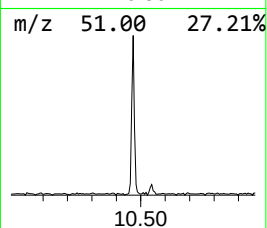
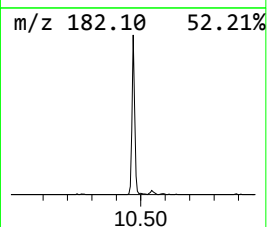
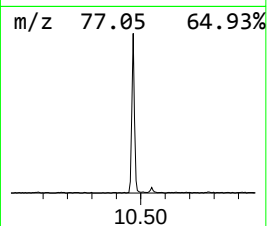
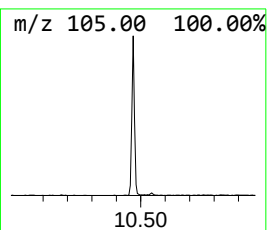
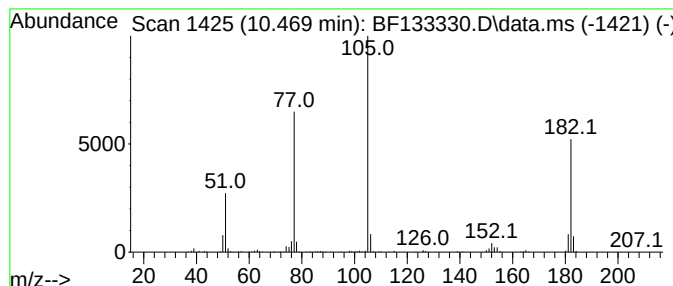
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	2.77 ng	272287	Acenaphthene-d10	9.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3			Benzoyl bromide	184	C7H5BrO	000618-32-6	47
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47



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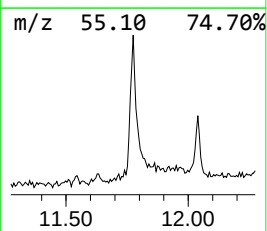
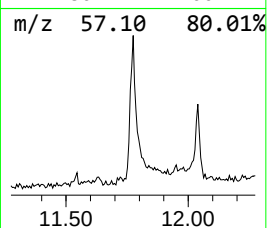
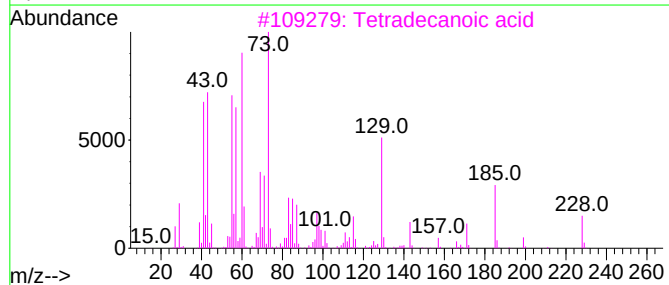
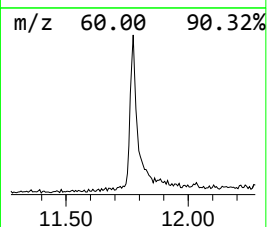
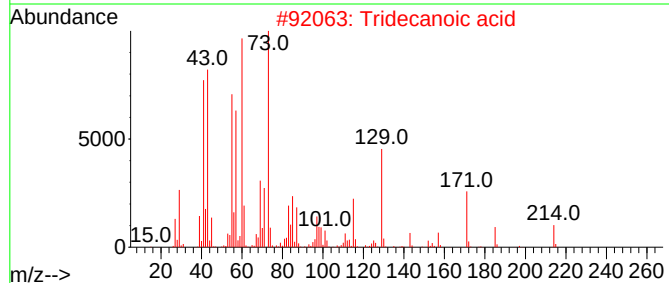
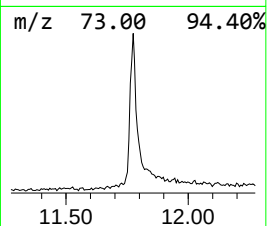
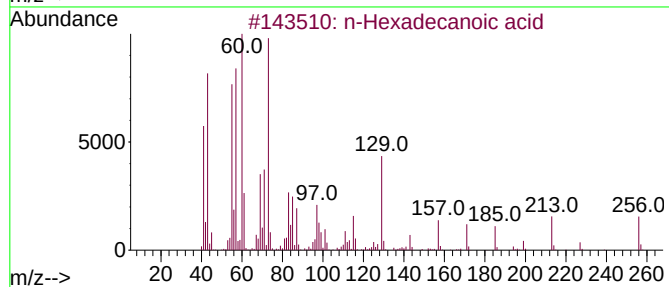
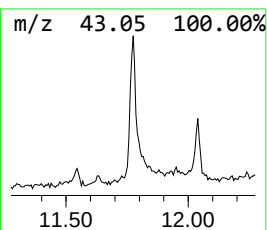
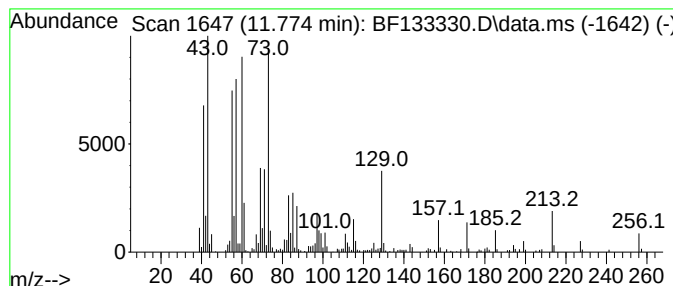
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.775	3.95 ng	388548	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78



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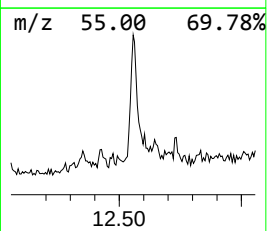
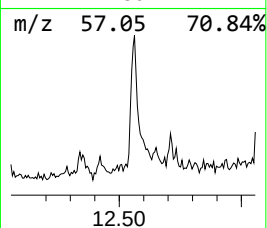
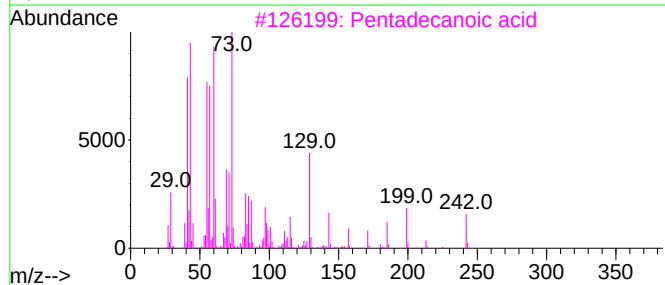
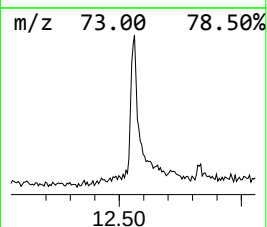
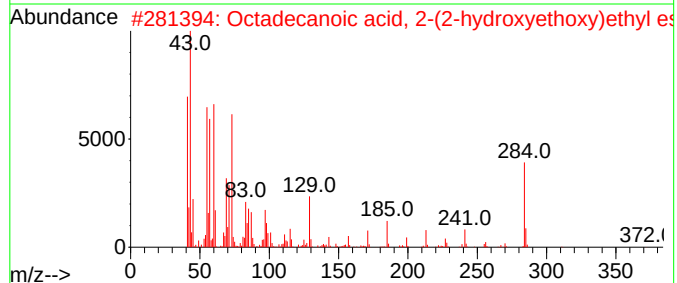
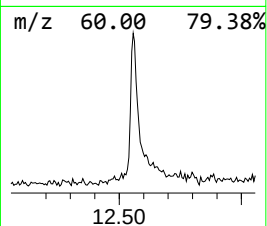
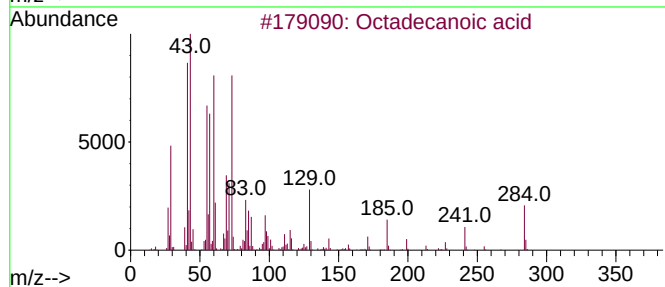
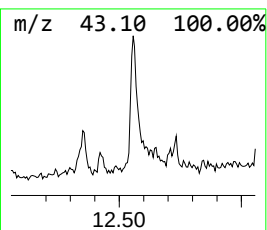
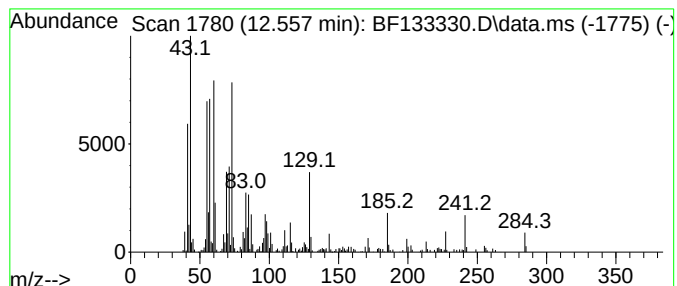
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.557	7.44 ng	437909	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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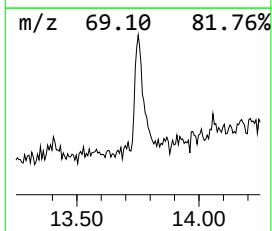
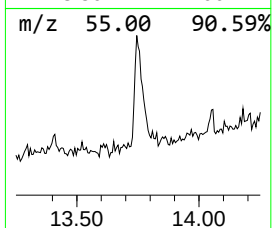
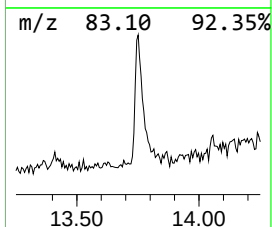
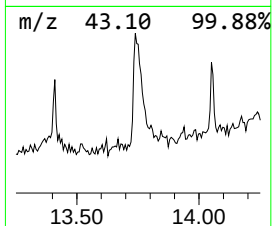
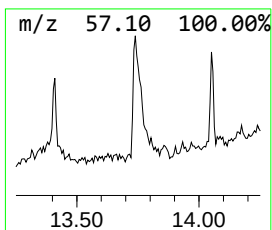
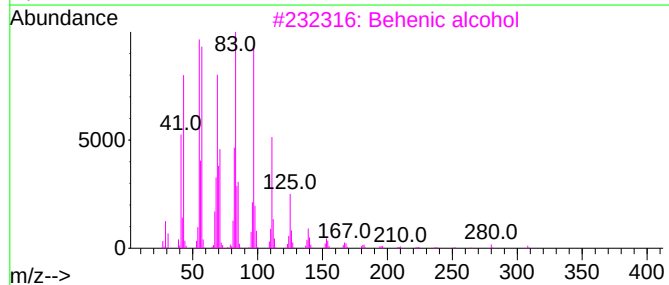
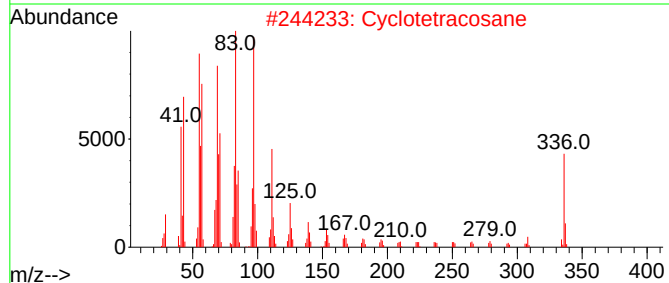
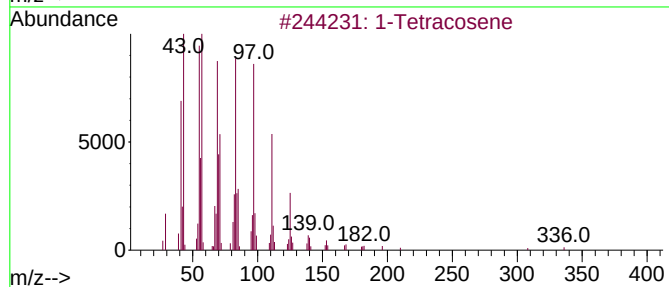
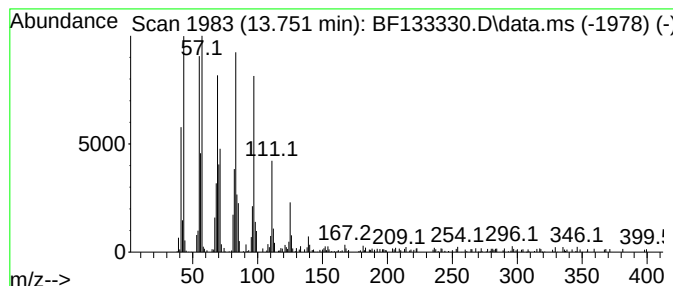
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Tetracosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	6.37 ng	374685	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetracosene	336	C24H48	010192-32-2	99
2			Cyclotetracosane	336	C24H48	000297-03-0	98
3			Behenic alcohol	326	C22H46O	000661-19-8	95
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	95
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051023\
Data File : BF133330.D
Acq On : 10 May 2023 14:55
Operator : CG\JU
Sample : 02719-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04_0-2_20230509

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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-...	4.916	29.5	ng	1834550	1	6.722	1242130	20.0
2-Pentanone, 4-...	5.728	2.5	ng	154063	1	6.722	1242130	20.0
Benzophenone	10.469	2.8	ng	272287	3	9.757	1966210	20.0
n-Hexadecanoic ...	11.775	4.0	ng	388548	4	11.239	1965500	20.0
Octadecanoic acid	12.557	7.4	ng	437909	5	13.874	1176810	20.0
1-Tetracosene	13.751	6.4	ng	374685	5	13.874	1176810	20.0