

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
 Data File : BF133850.D
 Acq On : 20 Jun 2023 11:48
 Operator : CG\JU
 Sample : 03282-06
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-NEX-002

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-BF060923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133850.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	4	9	20	rVB	424495	548693	42.33%	3.990%
2	2.252	24	28	35	rVB	22524	34853	2.69%	0.253%
3	3.963	314	319	323	rVB	15447	19960	1.54%	0.145%
4	5.087	506	510	516	rBV	165327	180519	13.92%	1.313%
5	5.487	574	578	588	rBV	1393820	1278309	98.61%	9.295%
6	6.492	744	749	752	rBV	1404338	1296367	100.00%	9.427%
7	6.857	807	811	814	rBV	713046	563336	43.45%	4.096%
8	7.416	902	906	909	rBV	1096925	854247	65.90%	6.212%
9	8.133	1025	1028	1032	rBV	866820	711984	54.92%	5.177%
10	9.210	1207	1211	1215	rBV	1307123	1038896	80.14%	7.554%
11	9.480	1250	1257	1264	rBV7	11114	23554	1.82%	0.171%
12	9.816	1309	1314	1324	rVB3	16334	31076	2.40%	0.226%
13	9.892	1324	1327	1331	rBV	934154	733976	56.62%	5.337%
14	10.098	1357	1362	1367	rBV5	19082	30893	2.38%	0.225%
15	10.304	1393	1397	1405	rVB2	13535	26104	2.01%	0.190%
16	10.610	1444	1449	1452	rBV	111807	99757	7.70%	0.725%
17	10.680	1458	1461	1465	rBV	728847	685953	52.91%	4.988%
18	10.922	1499	1502	1505	rBV	22190	19201	1.48%	0.140%
19	11.386	1577	1581	1584	rBV	827463	660894	50.98%	4.806%
20	11.845	1655	1659	1661	rBV4	17612	24455	1.89%	0.178%
21	11.916	1664	1671	1688	rVB2	414843	690418	53.26%	5.020%
22	12.610	1786	1789	1790	rBV2	23643	23947	1.85%	0.174%
23	12.651	1790	1796	1801	rVV2	144184	311730	24.05%	2.267%
24	12.710	1801	1806	1817	rVB	241416	425495	32.82%	3.094%
25	12.874	1830	1834	1848	rVB2	58648	110911	8.56%	0.806%
26	12.980	1848	1852	1857	rVB	746874	613005	47.29%	4.457%
27	13.216	1888	1892	1894	rBV2	19724	20960	1.62%	0.152%
28	13.833	1992	1997	2001	rBV	135632	224426	17.31%	1.632%
29	13.874	2001	2004	2006	rVV	179952	254462	19.63%	1.850%
30	13.910	2006	2010	2015	rVV	632488	923591	71.24%	6.716%
31	13.963	2015	2019	2026	rVB	40304	60652	4.68%	0.441%
32	14.045	2026	2033	2036	rBV	530514	544299	41.99%	3.958%
33	14.210	2058	2061	2064	rBV	22929	24541	1.89%	0.178%
34	14.521	2111	2114	2116	rVB	29206	28149	2.17%	0.205%
35	14.915	2178	2181	2184	rVB2	27395	28963	2.23%	0.211%
36	15.192	2225	2228	2234	rVB	31566	33773	2.61%	0.246%

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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-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.551	2284	2289	2293	rBV	446540	569877	43.96%	4.144%
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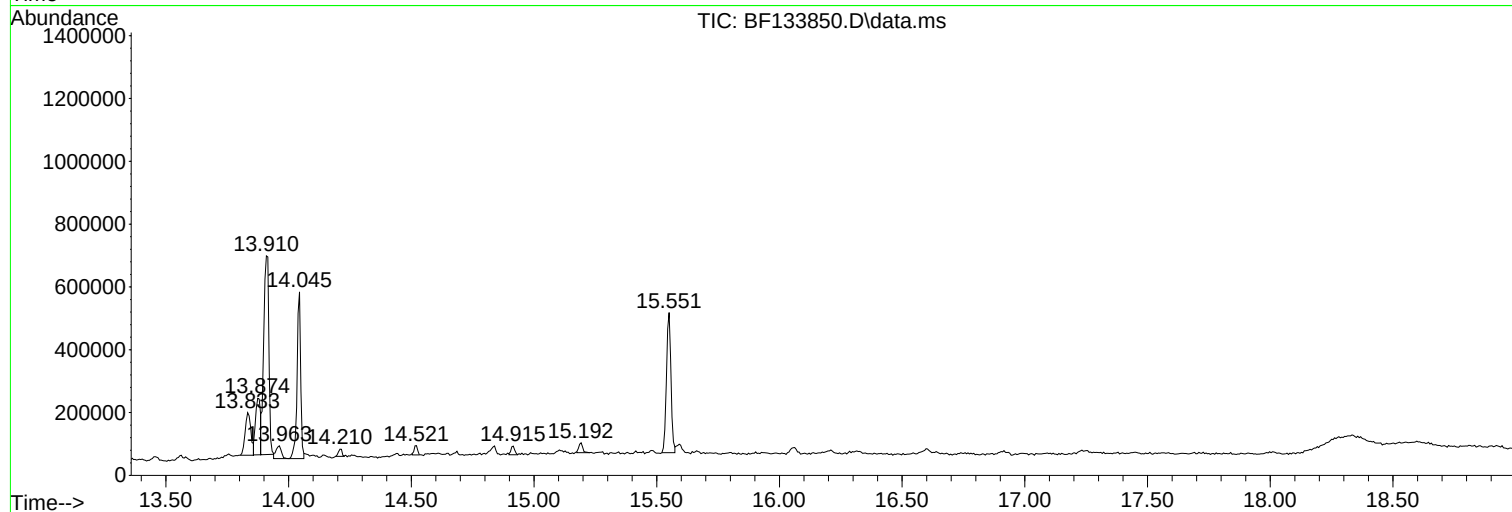
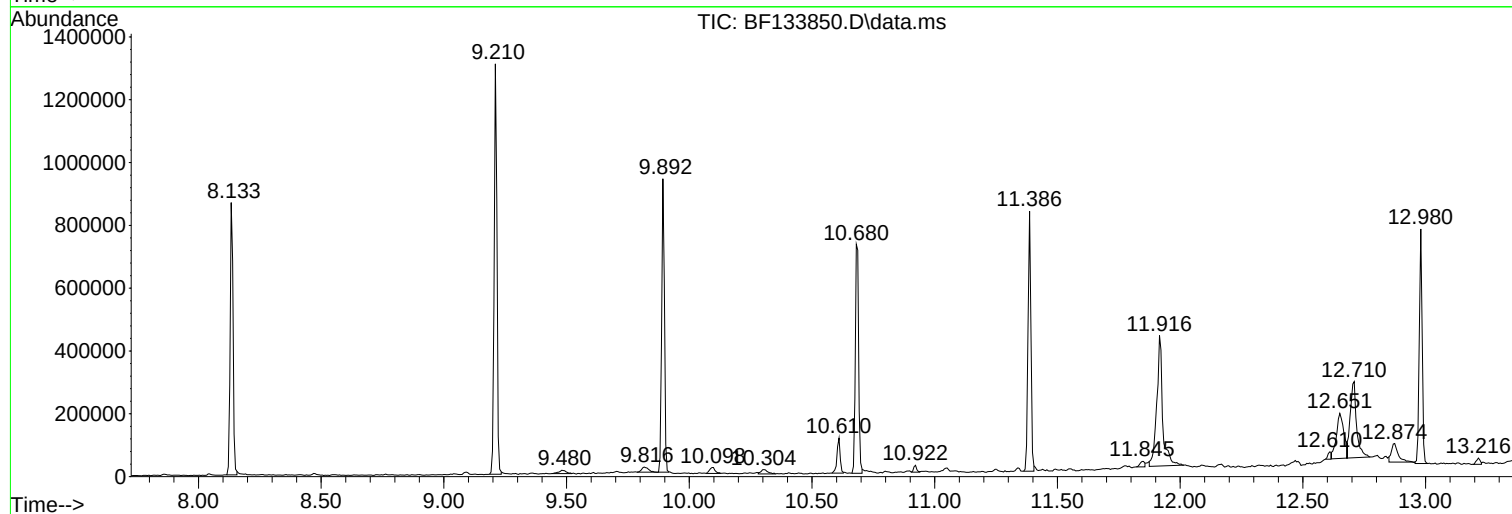
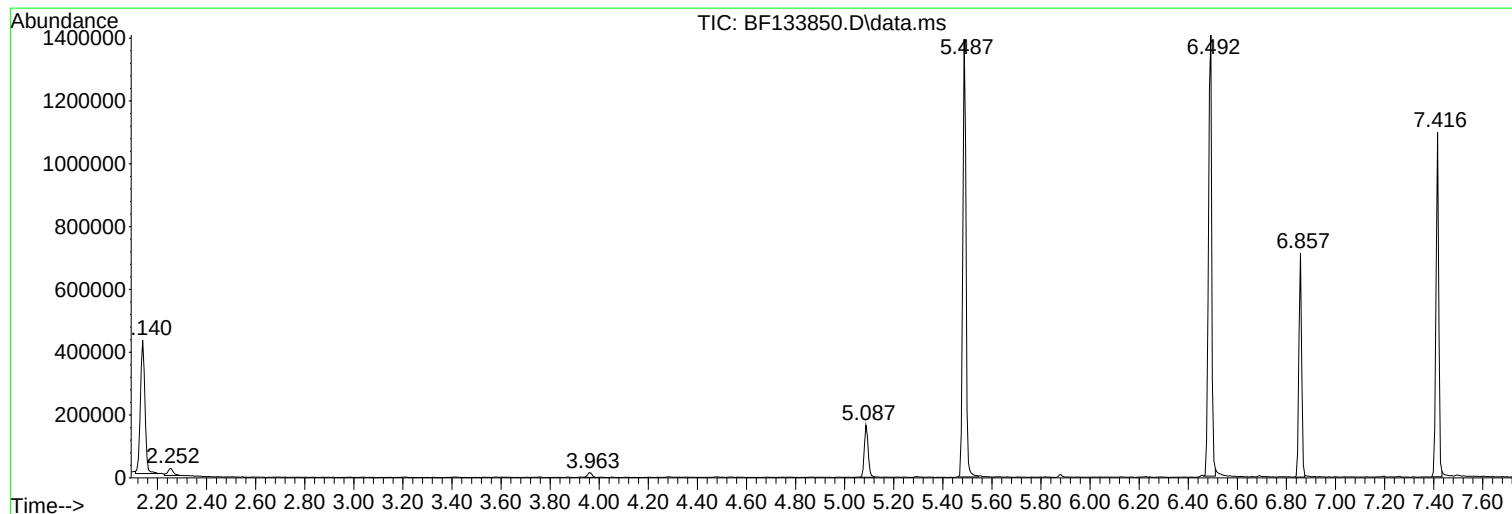
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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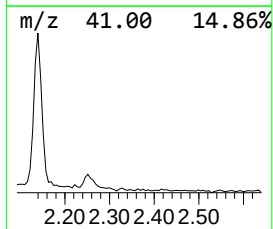
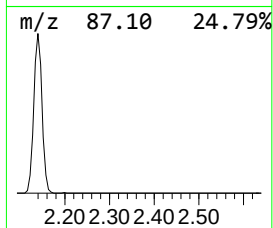
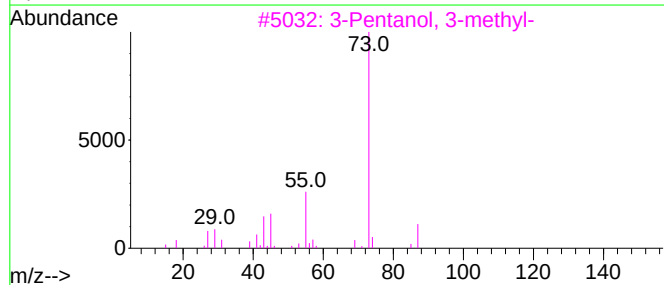
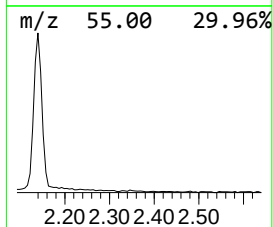
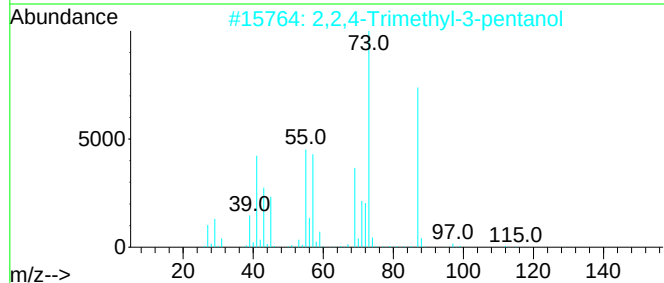
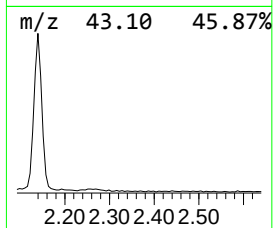
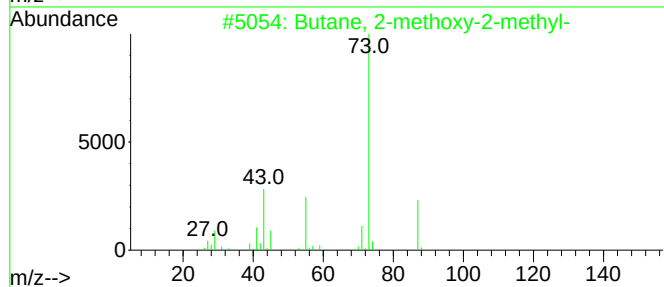
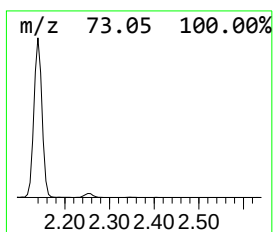
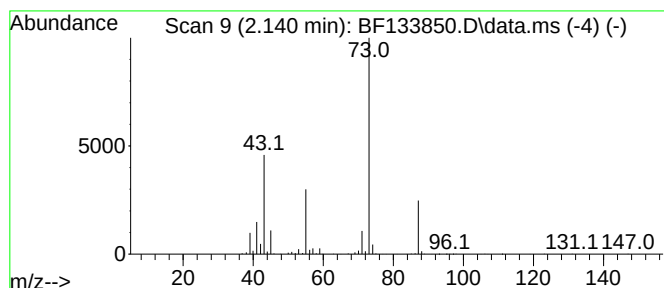
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	19.48 ng	548693	1,4-Dichlorobenzene-d4	6.857

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			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28



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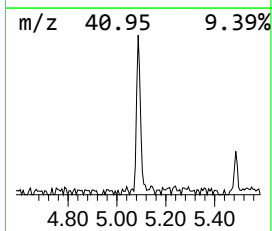
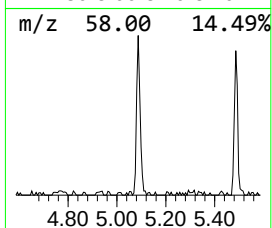
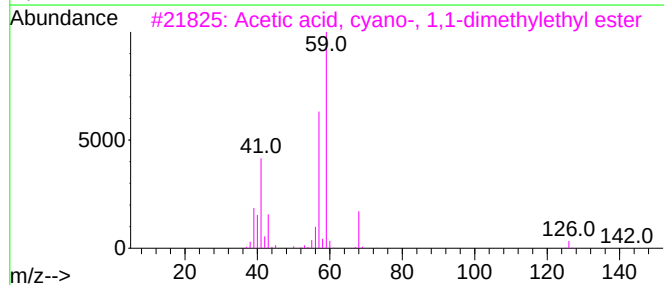
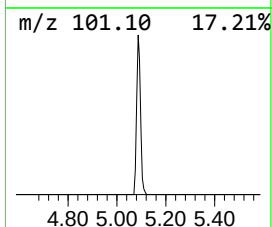
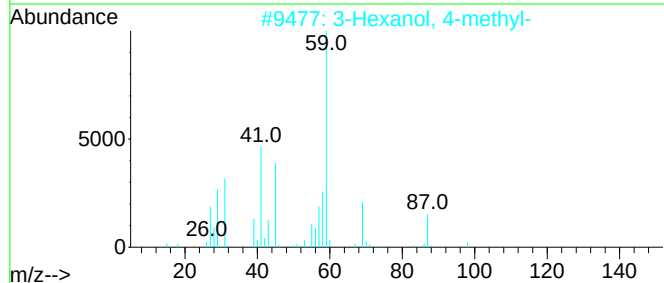
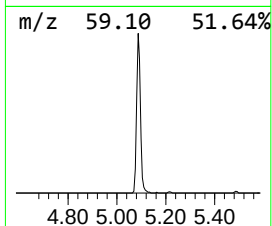
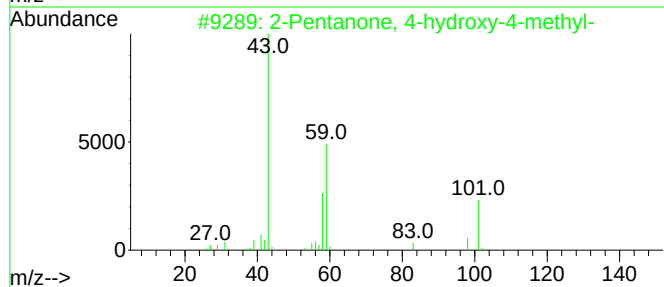
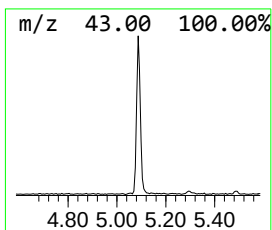
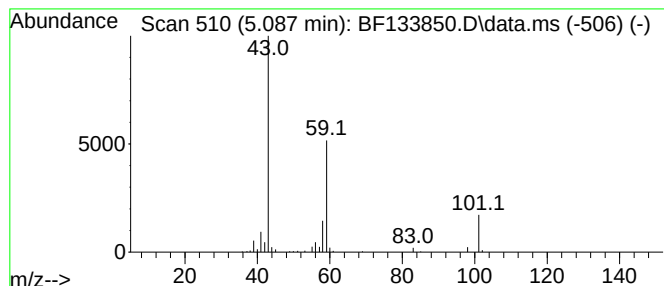
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	6.41 ng	180519	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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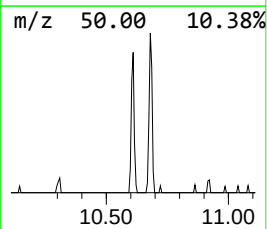
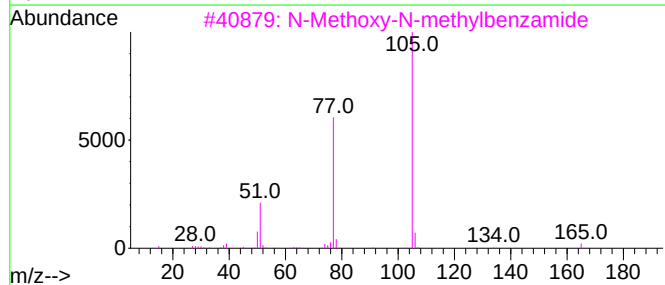
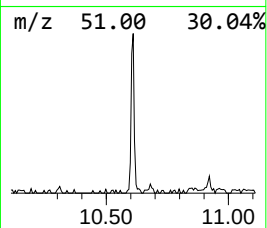
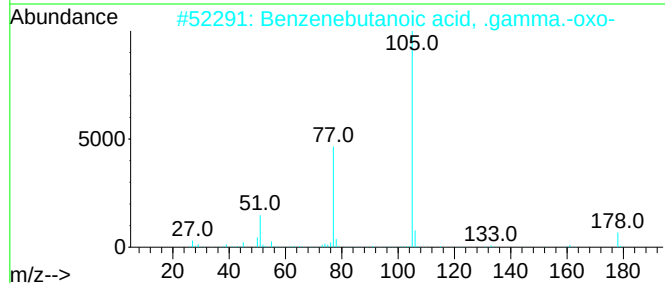
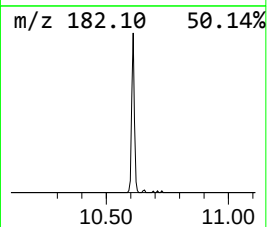
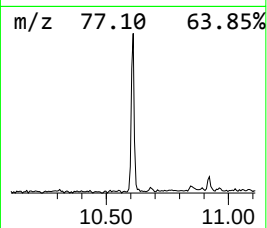
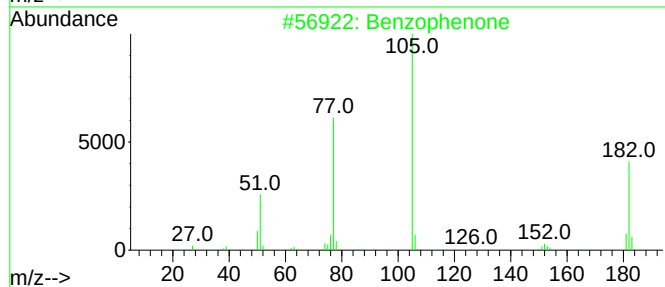
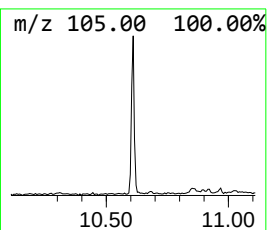
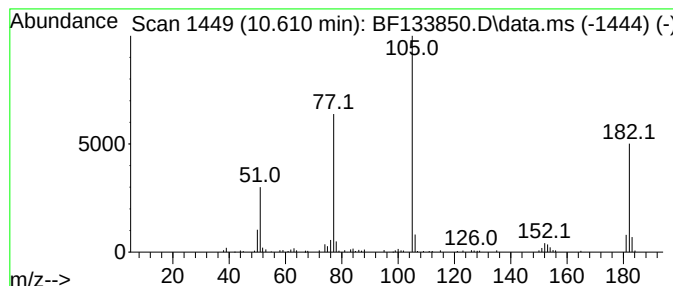
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.610	2.72 ng	99757	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5			Benzilamide	227	C14H13NO2	004746-87-6	47



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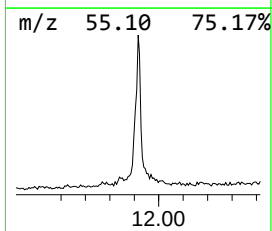
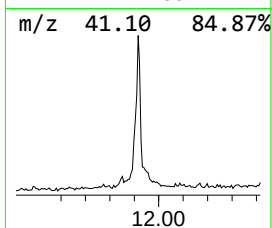
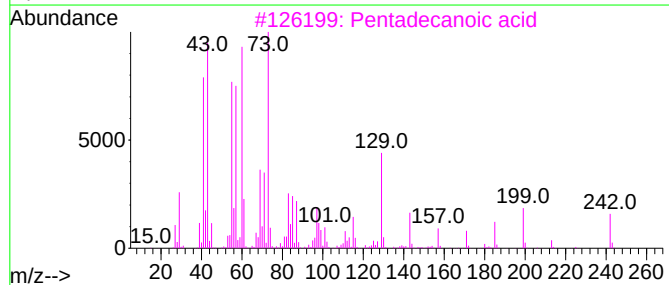
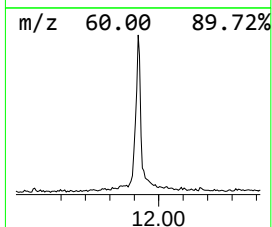
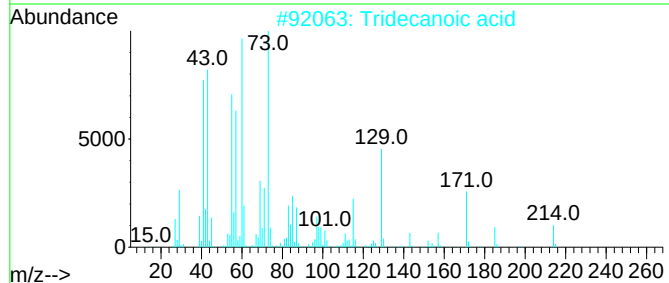
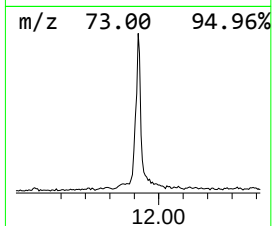
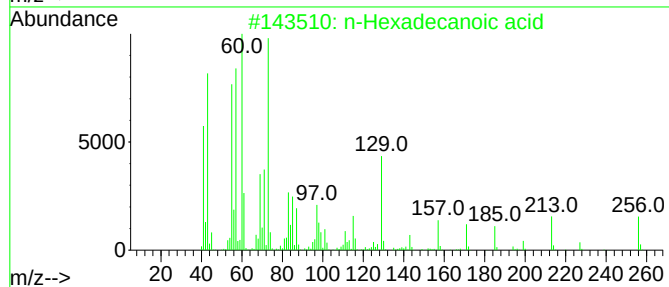
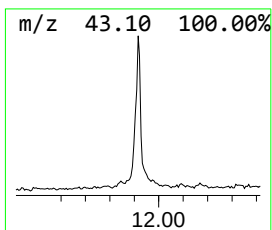
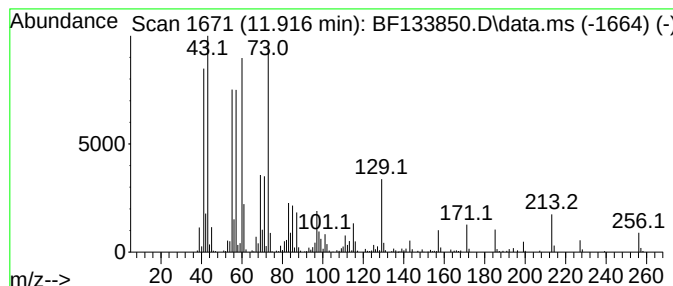
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	20.89 ng	690418	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	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Undecanoic acid	186	C11H22O2	000112-37-8	68



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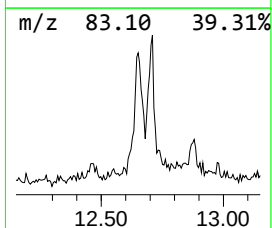
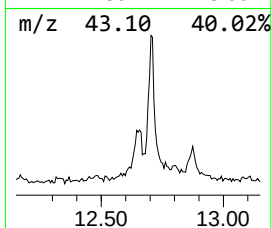
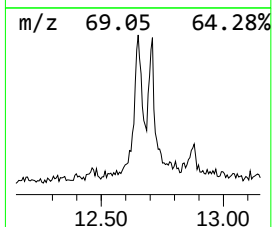
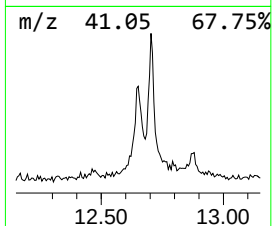
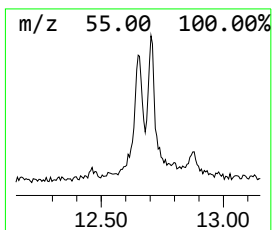
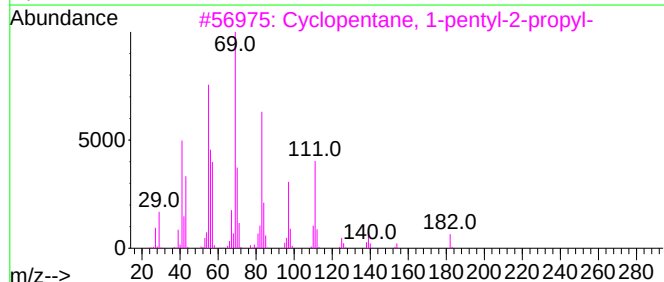
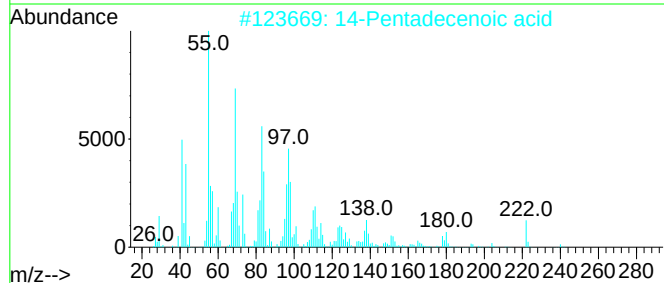
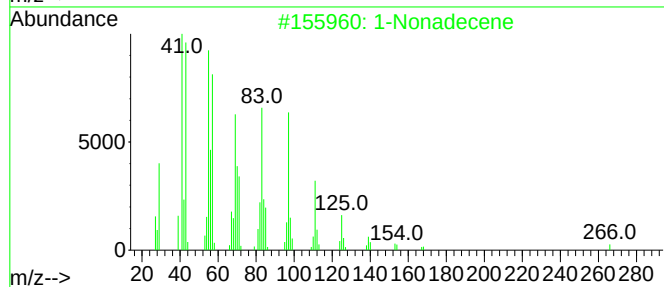
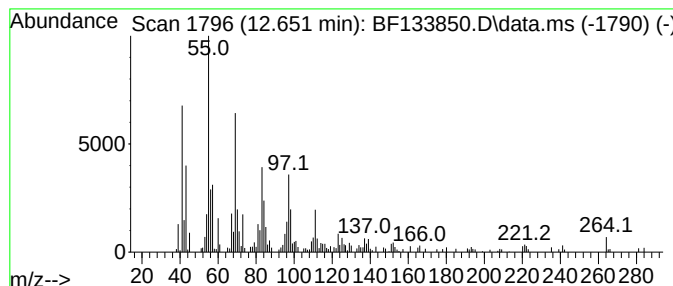
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.651	9.43 ng	311730	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	83
2	14-Pentadecenoic acid			240	C15H28O2	017351-34-7	72
3	Cyclopentane, 1-pentyl-2-propyl-			182	C13H26	062199-51-3	43
4	9-Octadecenoic acid, (E)-			282	C18H34O2	000112-79-8	43
5	Cyclohexane, 1,1'-[3-(2-cyclopen...			346	C25H46	055401-71-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133850.D
Acq On : 20 Jun 2023 11:48
Operator : CG\JU
Sample : 03282-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
WC-NEX-002

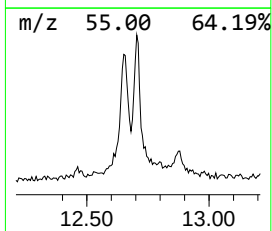
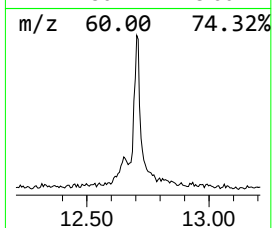
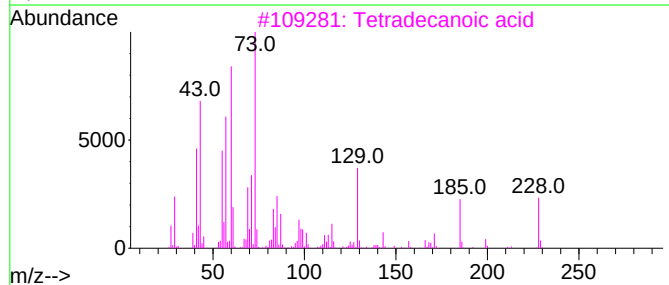
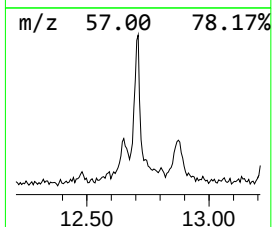
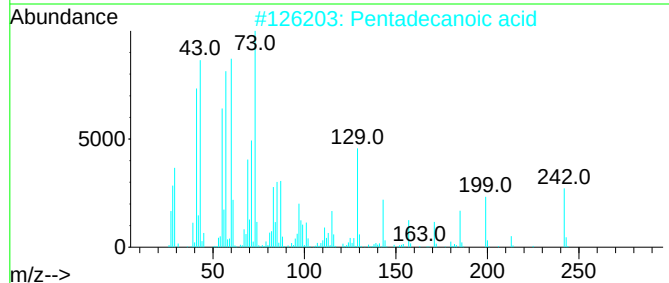
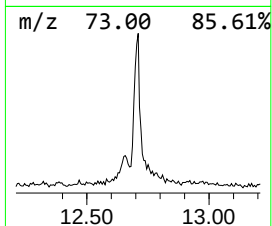
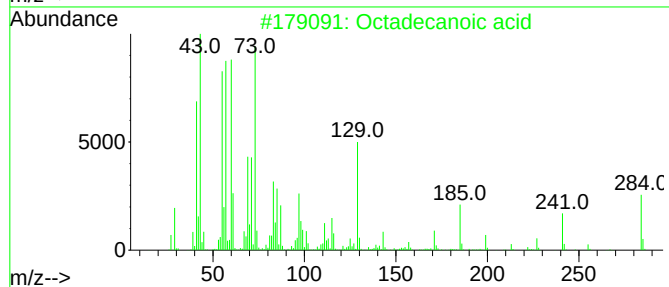
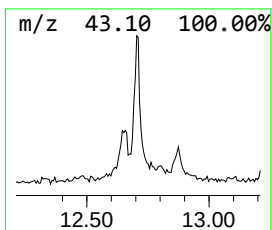
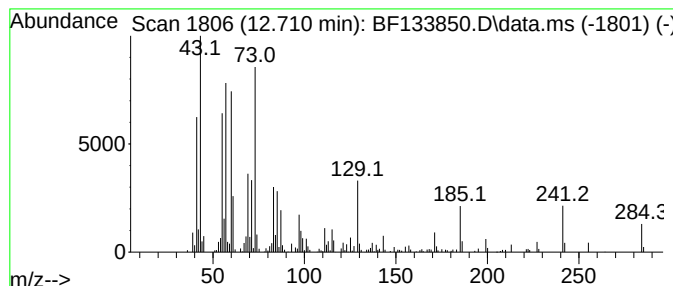
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	12.88 ng	425495	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4			n-Decanoic acid	172	C10H20O2	000334-48-5	60
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133850.D
Acq On : 20 Jun 2023 11:48
Operator : CG\JU
Sample : 03282-06
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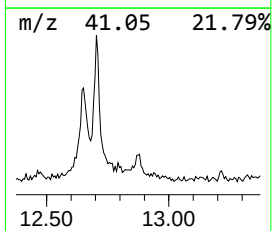
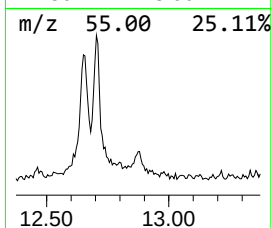
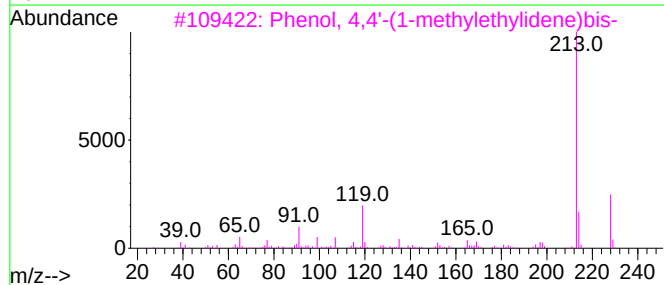
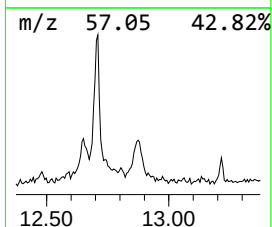
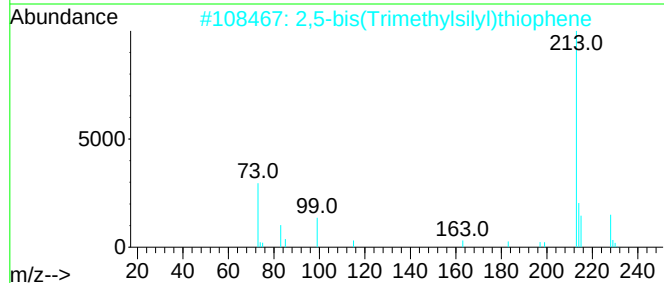
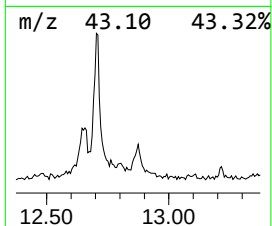
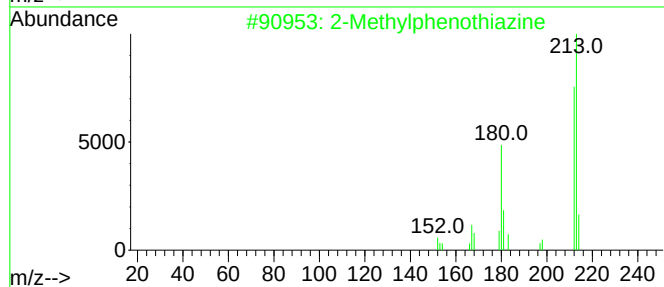
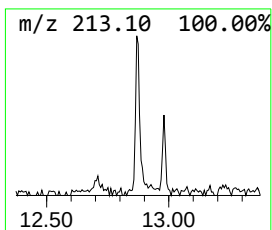
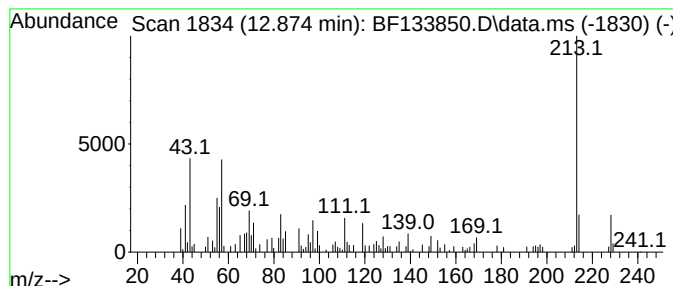
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Methylphenothiazine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.874	4.08 ng	110911	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methylphenothiazine	213	C13H11NS	005828-51-3	72
2			2,5-bis(Trimethylsilyl)thiophene	228	C10H20SSi2	017906-71-7	59
3			Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	000080-05-7	58
4			2-Trimethylsilyl-3-trimethylsilyl-5-methylthiophene	228	C8H20N4Si2	1000373-05-5	50
5			2H,8H-Benzo[1,2-b:3,4-b']dipyran-5-one	228	C14H12O3	000523-59-1	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133850.D
Acq On : 20 Jun 2023 11:48
Operator : CG\JU
Sample : 03282-06
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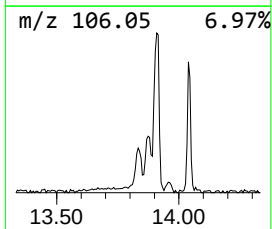
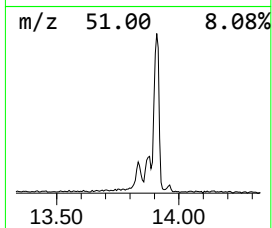
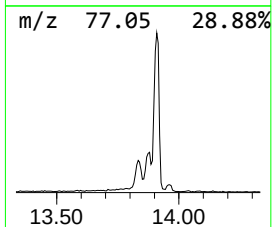
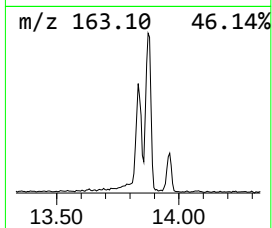
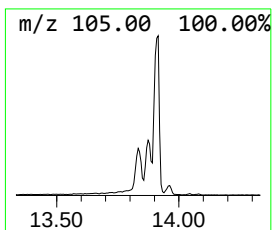
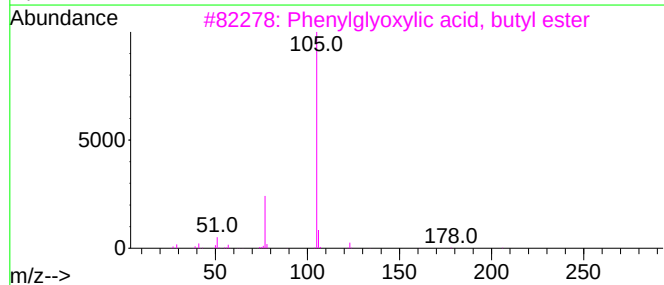
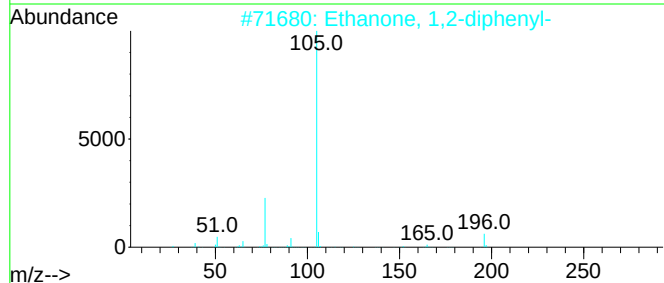
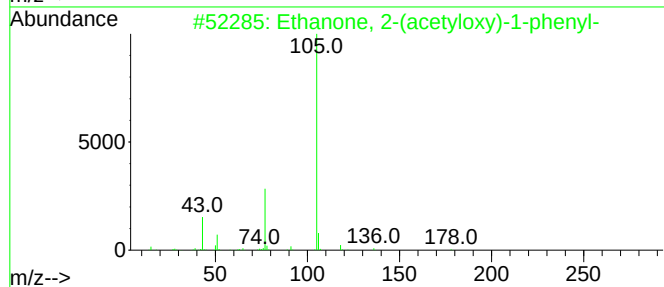
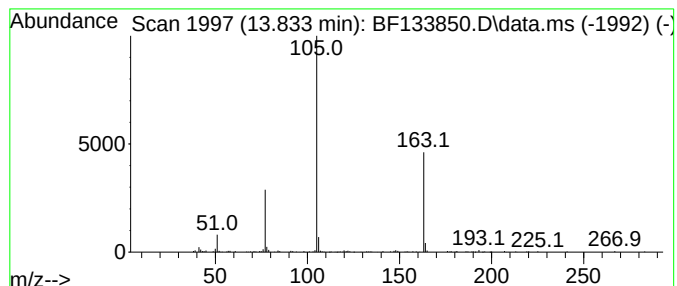
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown13.833 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	8.25 ng	224426	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 2-(acetyloxy)-1-phenyl-	178	C10H10O3	002243-35-8	43
2			Ethanone, 1,2-diphenyl-	196	C14H12O	000451-40-1	43
3			Phenylglyoxylic acid, butyl ester	206	C12H14O3	1000453-46-6	38
4			2,3,4-O-Tribenzoyl-1-ribose...	464	C26H21F07	1000129-81-2	38
5			2-Benzamido-4,4'-dinitrodiphenyl...	427	C19H13N3O7S	1000255-05-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133850.D
Acq On : 20 Jun 2023 11:48
Operator : CG\JU
Sample : 03282-06
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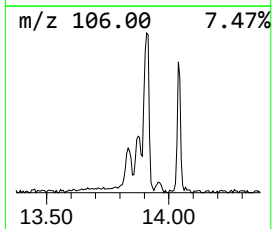
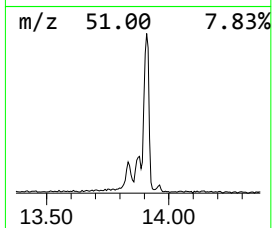
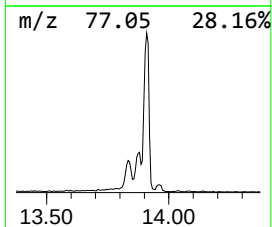
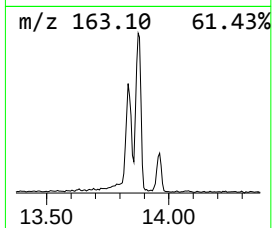
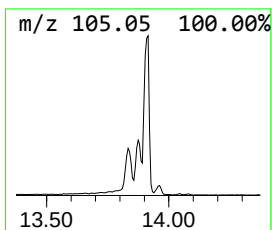
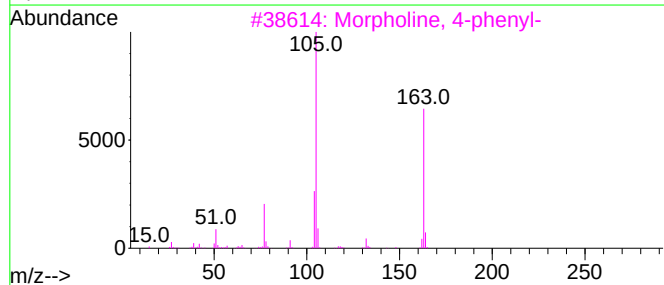
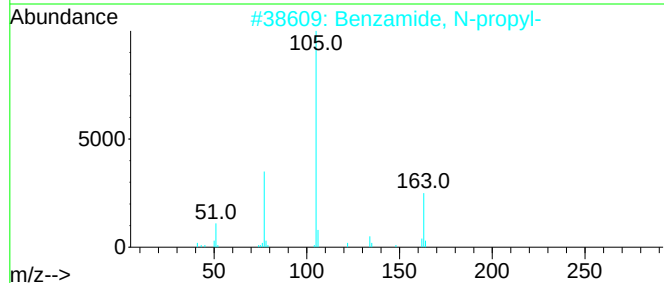
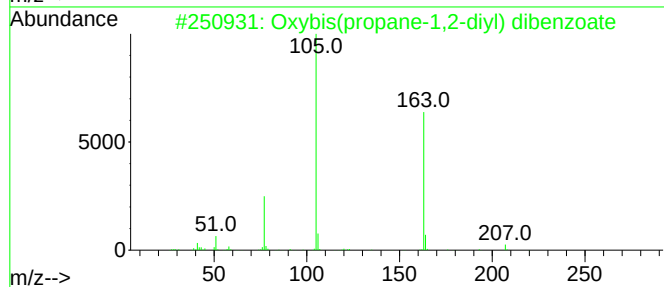
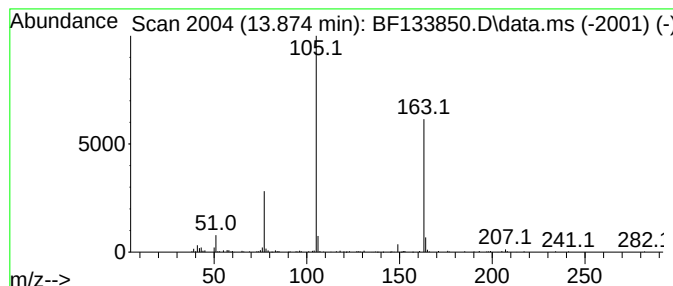
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Oxybis(propene-1,2-diyl) di... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	9.35 ng	254462	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	80
2			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	72
3			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	59
4			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	35
5			2-Bromoisobutyrophenone	226	C10H11BrO	010409-54-8	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133850.D
Acq On : 20 Jun 2023 11:48
Operator : CG\JU
Sample : 03282-06
Misc :
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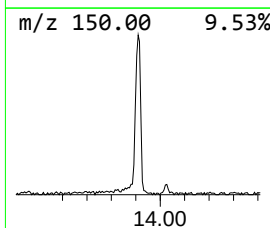
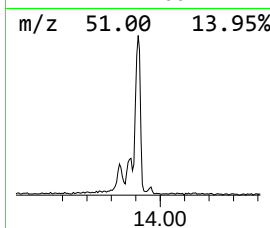
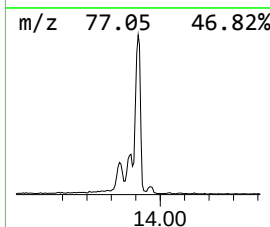
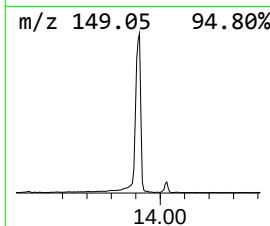
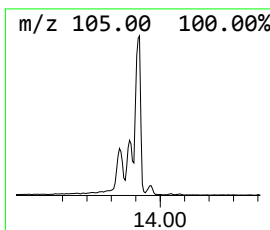
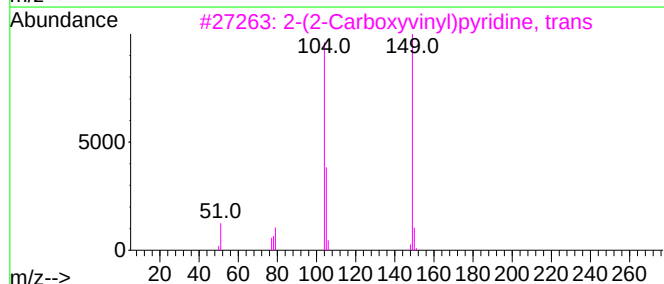
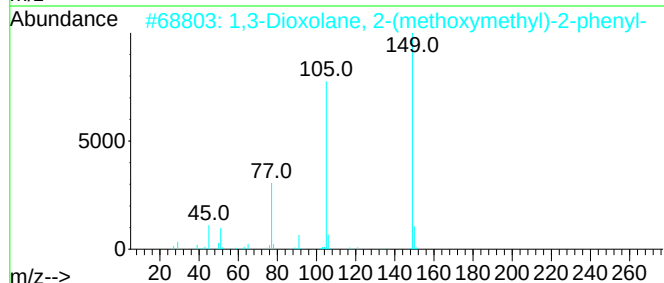
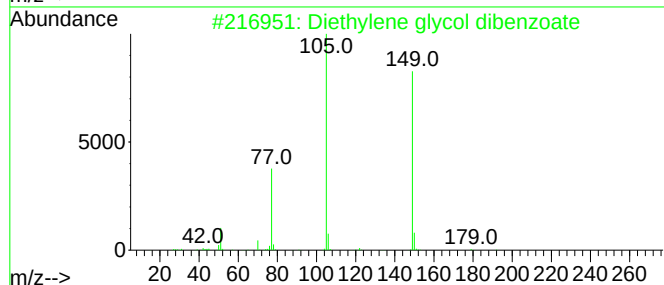
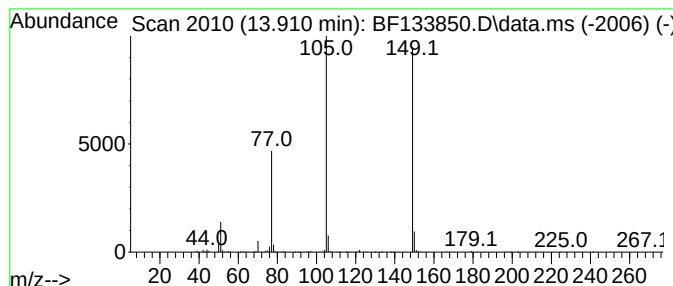
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	33.94 ng	923591	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	72
3			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	53
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	35
5			Benzoic acid 5-methyl-2-phenyl-2...	278	C17H14N2O2	056159-67-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
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Acq On : 20 Jun 2023 11:48
Operator : CG\JU
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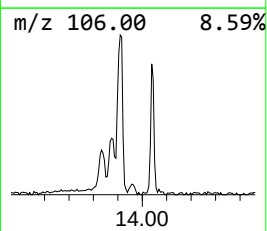
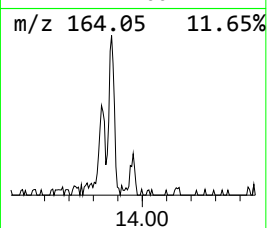
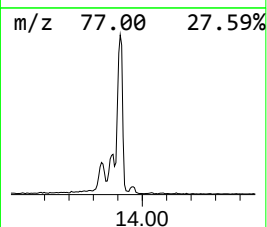
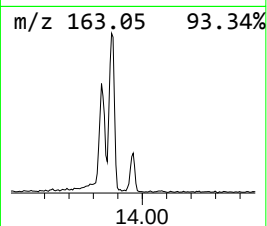
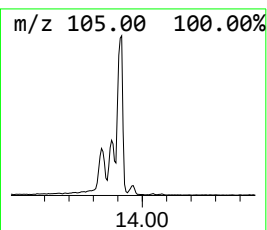
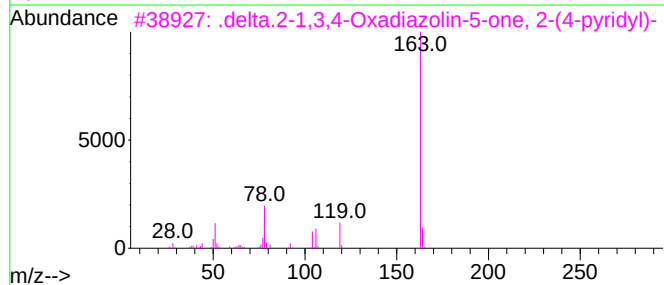
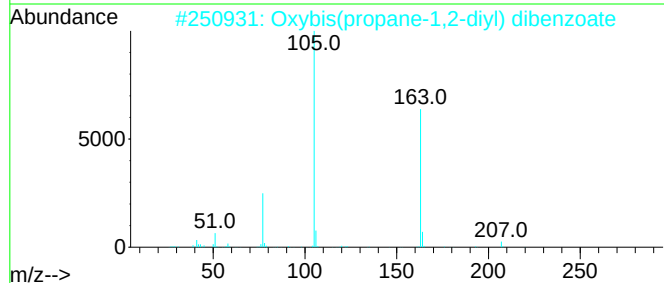
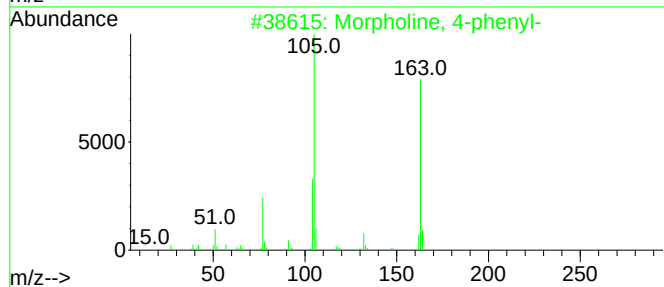
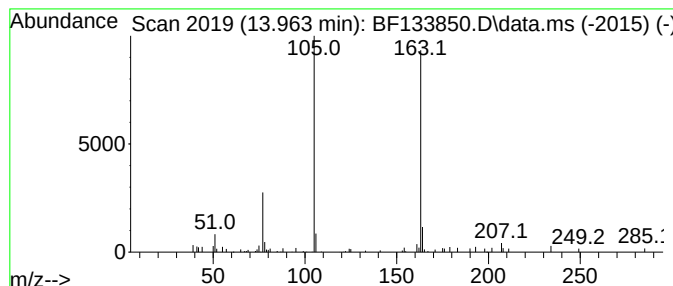
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Morpholine, 4-phenyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.963	2.23 ng	60652	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	80
2			Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	78
3			.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	47
4			Propanoic acid, 2-(benzoylamino)...	251	C13H17NO4	141627-52-3	14
5			Hippuric acid, methyl ester	193	C10H11NO3	001205-08-9	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062023\
Data File : BF133850.D
Acq On : 20 Jun 2023 11:48
Operator : CG\JU
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
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2-Pentanone, 4-...	5.087	6.4	ng	180519	1	6.857	563336	20.0
Benzophenone	10.610	2.7	ng	99757	3	9.892	733976	20.0
n-Hexadecanoic ...	11.916	20.9	ng	690418	4	11.386	660894	20.0
1-Nonadecene	12.651	9.4	ng	311730	4	11.386	660894	20.0
Octadecanoic acid	12.710	12.9	ng	425495	4	11.386	660894	20.0
2-Methylphenoth...	12.874	4.1	ng	110911	5	14.045	544299	20.0
unknown13.833	13.833	8.3	ng	224426	5	14.045	544299	20.0
Oxybis(propane-...	13.874	9.3	ng	254462	5	14.045	544299	20.0
Diethylene glyc...	13.910	33.9	ng	923591	5	14.045	544299	20.0
Morpholine, 4-p...	13.963	2.2	ng	60652	5	14.045	544299	20.0