

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
 Data File : BF140158.D
 Acq On : 30 Oct 2024 15:34
 Operator : RC/JU
 Sample : P4611-13
 Misc :
 ALS Vial : 8 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-BF101824.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140158.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	5	12	22	rVB	1180239	1844009	66.24%	9.043%
2	5.104	505	512	520	rVB	48368	79387	2.85%	0.389%
3	5.498	573	579	584	rBV	1660686	2190013	78.66%	10.739%
4	6.504	743	750	755	rBV	1616035	2312903	83.08%	11.342%
5	6.881	809	814	819	rBV	496668	601354	21.60%	2.949%
6	7.439	903	909	914	rBV	1219711	1584317	56.91%	7.769%
7	7.692	948	952	963	rBV	43114	54499	1.96%	0.267%
8	8.163	1026	1032	1037	rBV	622991	775012	27.84%	3.801%
9	9.239	1209	1215	1220	rBV	2186850	2783981	100.00%	13.652%
10	9.922	1325	1331	1336	rBV	700270	858587	30.84%	4.210%
11	10.639	1447	1453	1460	rBV	483658	596832	21.44%	2.927%
12	10.716	1460	1466	1480	rVV	1247846	1672847	60.09%	8.203%
13	10.945	1501	1505	1515	rVB	43728	56989	2.05%	0.279%
14	11.416	1580	1585	1590	rBV	655002	828947	29.78%	4.065%
15	11.945	1670	1675	1698	rBV	291334	512473	18.41%	2.513%
16	12.733	1804	1809	1818	rBV	54754	99836	3.59%	0.490%
17	13.010	1850	1856	1861	rBV	1852888	2425574	87.13%	11.895%
18	13.927	2007	2012	2032	rBV	52983	159313	5.72%	0.781%
19	14.080	2033	2038	2047	rVB	344764	472013	16.95%	2.315%
20	15.615	2292	2299	2306	rBV	297484	483427	17.36%	2.371%

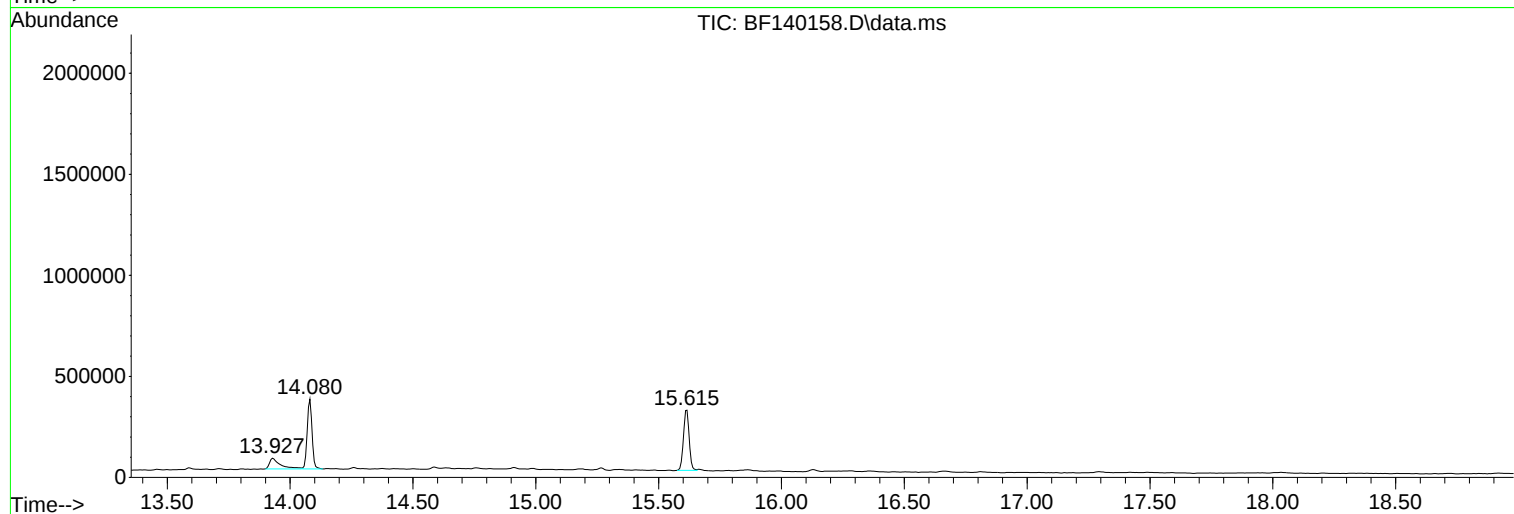
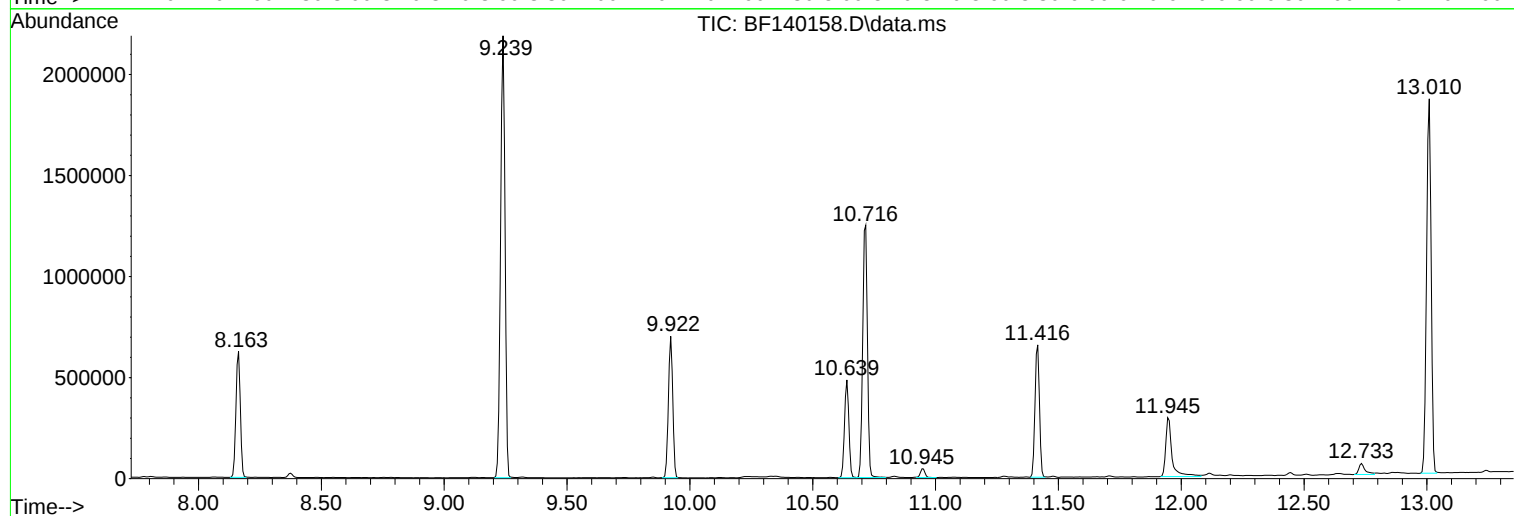
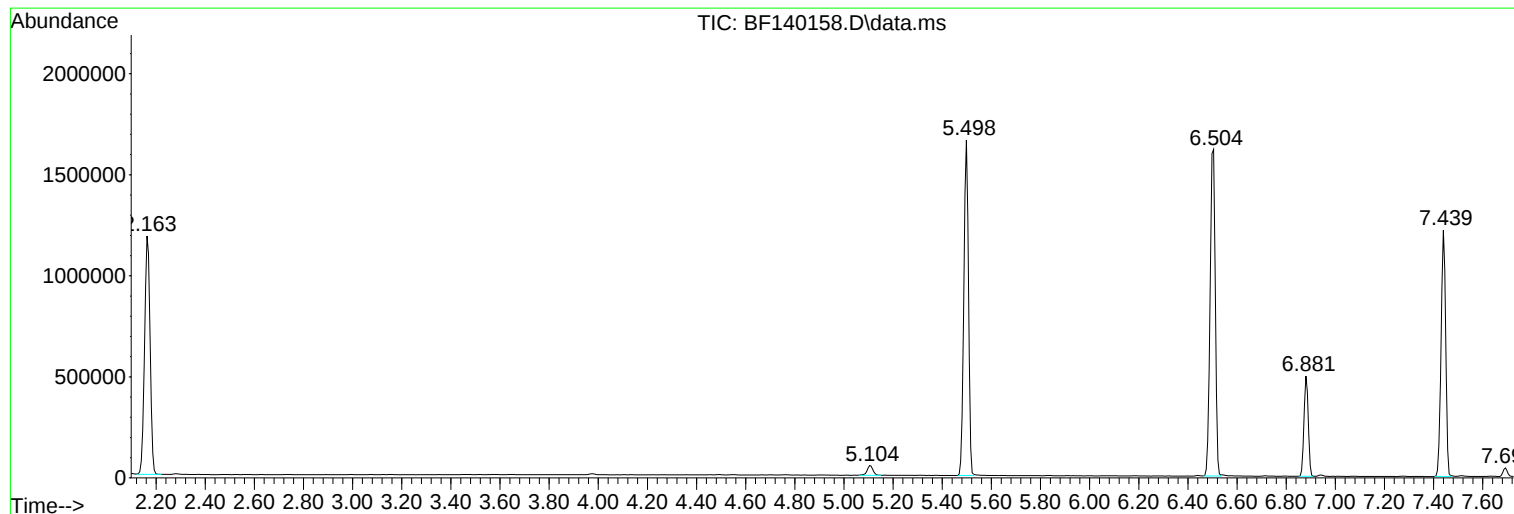
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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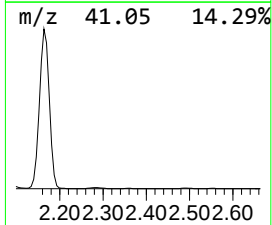
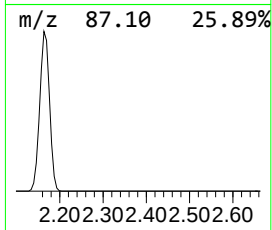
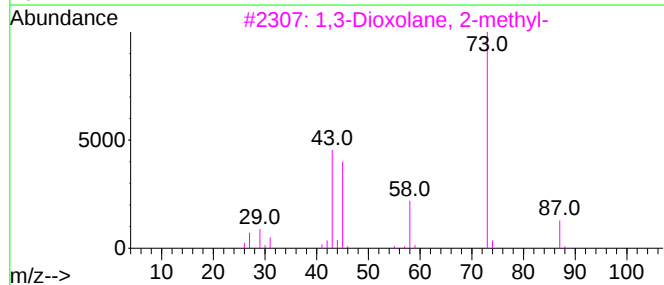
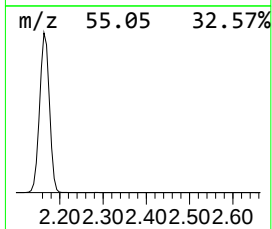
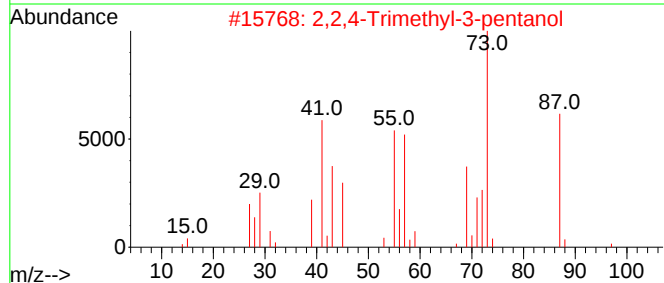
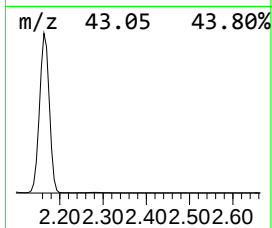
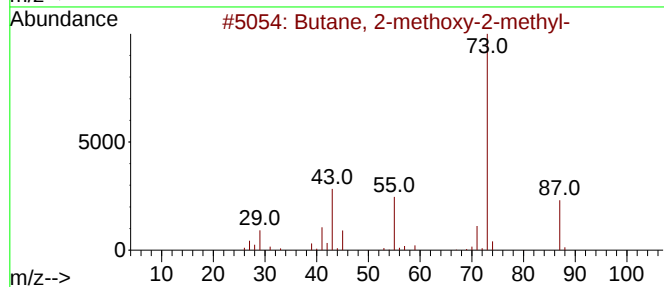
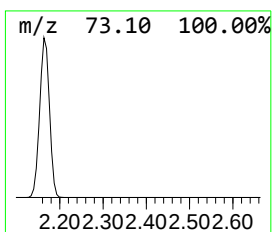
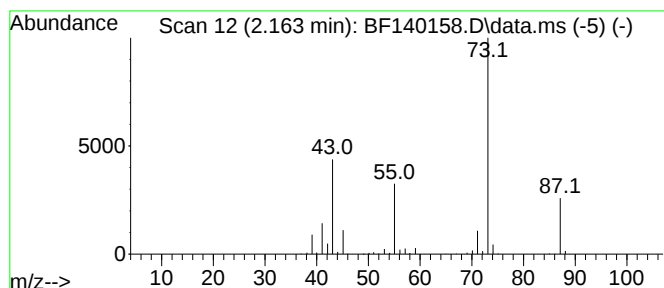
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.163	61.33 ng	1844010	1,4-Dichlorobenzene-d4	6.881

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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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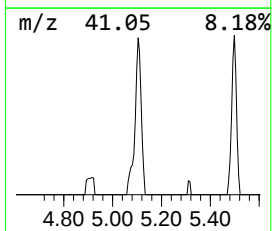
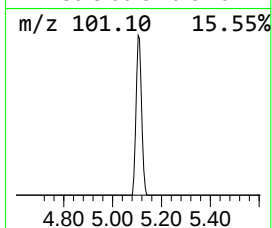
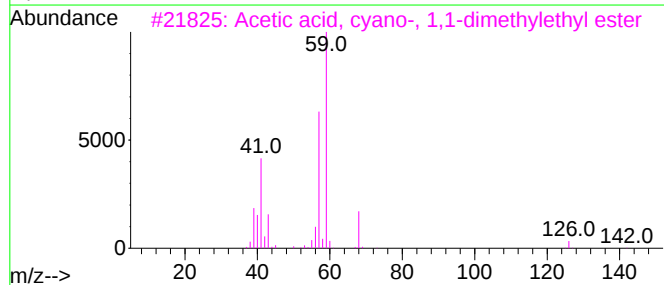
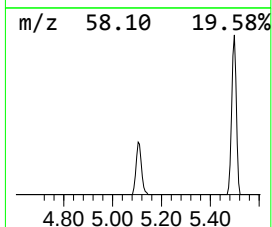
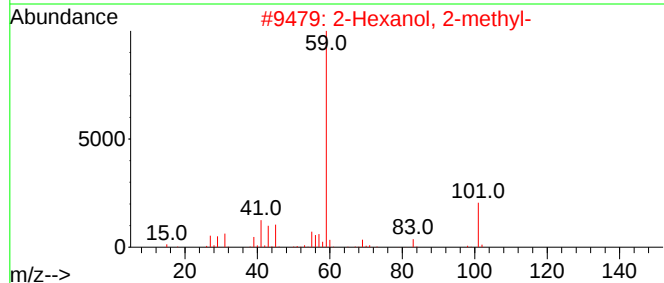
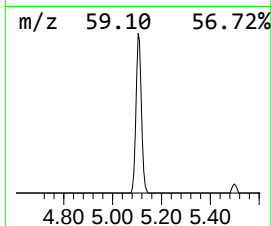
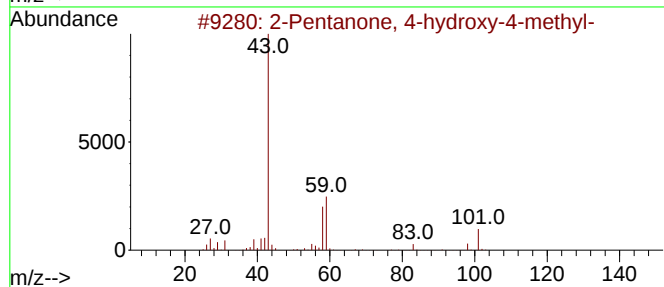
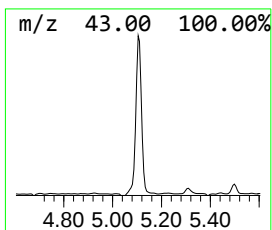
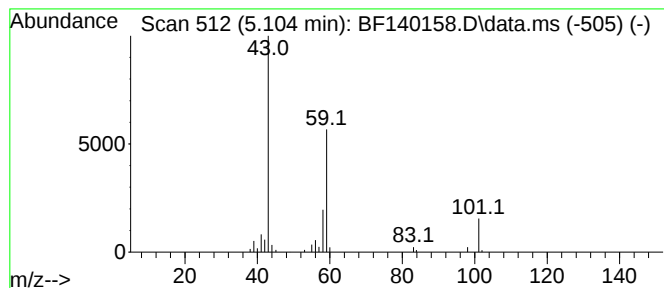
Instrument :
BNA_F
ClientSampleId :
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.104	2.64 ng	79387	1,4-Dichlorobenzene-d4	6.881	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	16



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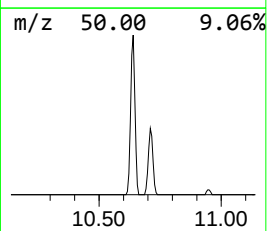
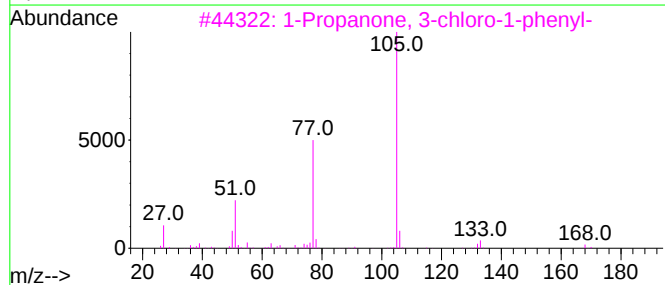
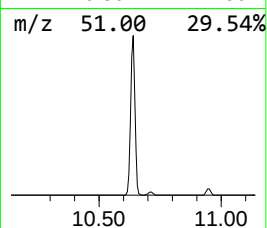
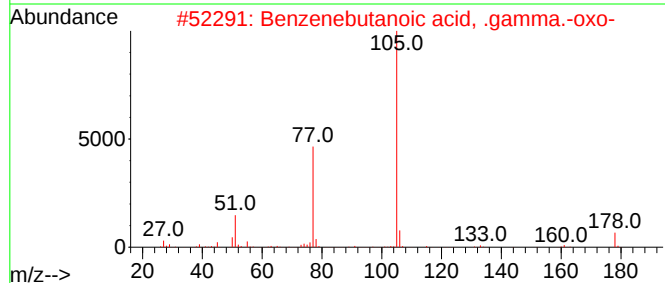
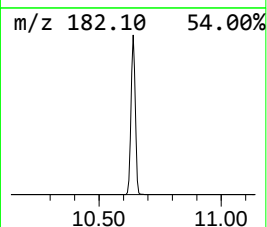
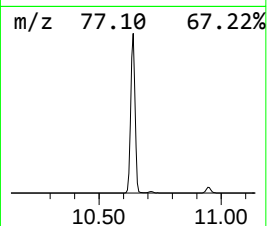
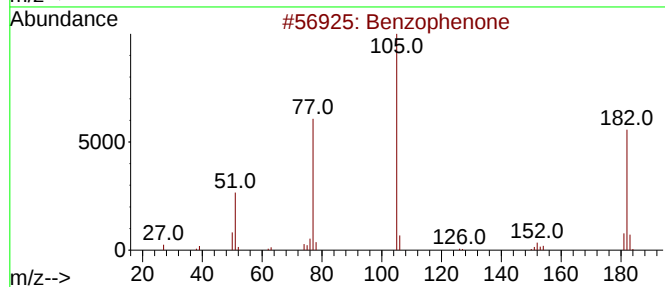
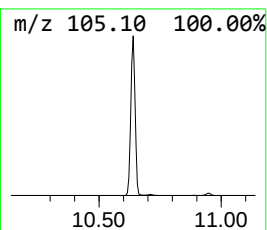
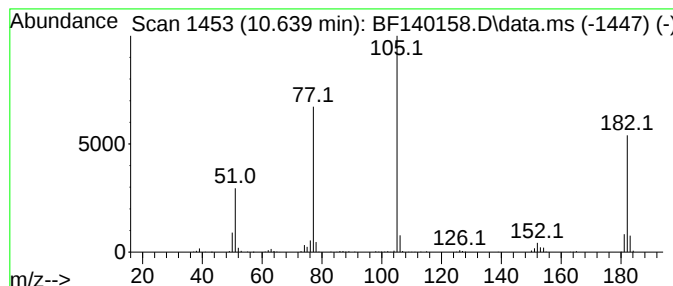
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Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.639	13.90 ng	596832	Acenaphthene-d10	9.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50
3			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	50
4			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	50
5			5-Oxo-5-phenylpentanenitrile	173	C11H11NO	1000486-83-7	50



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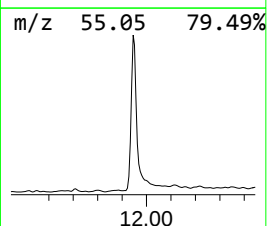
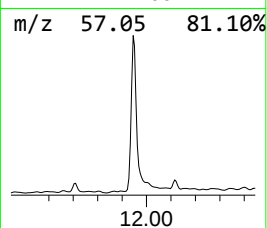
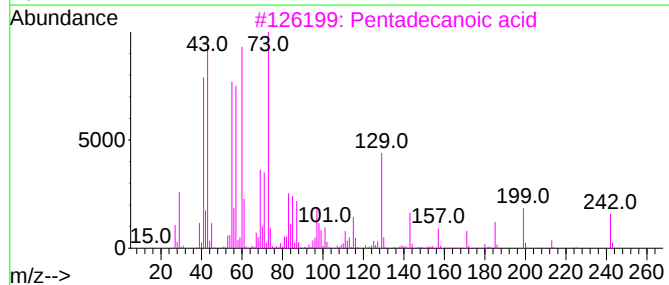
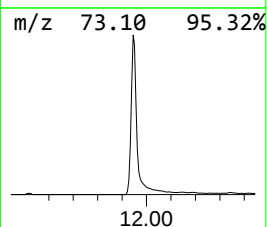
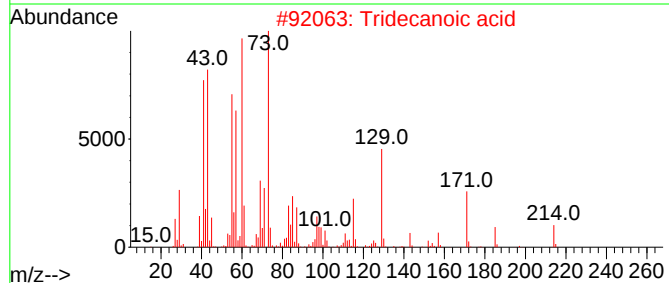
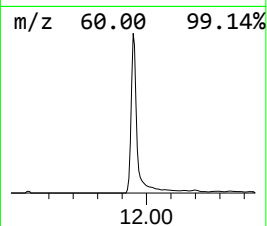
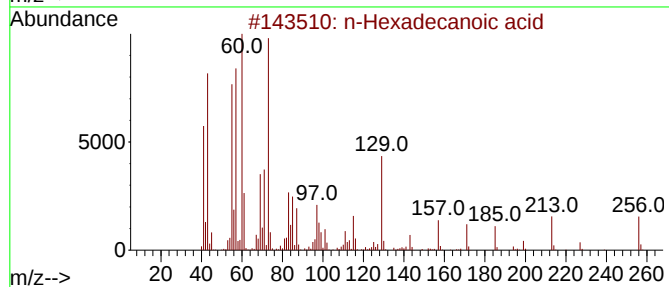
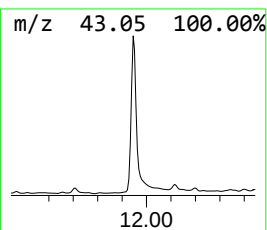
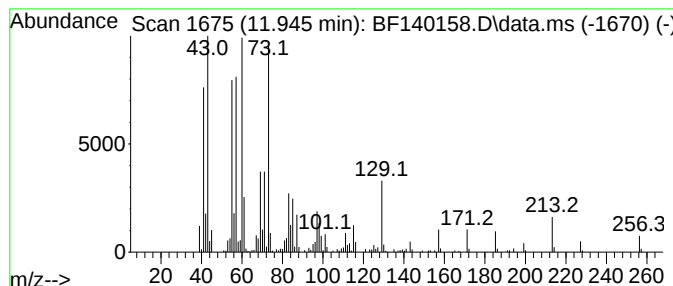
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	12.36 ng	512473	Phenanthrene-d10	11.416

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	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	78
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



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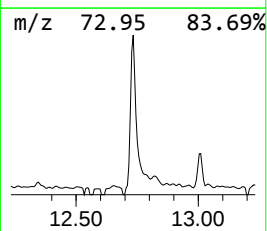
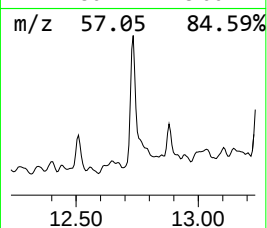
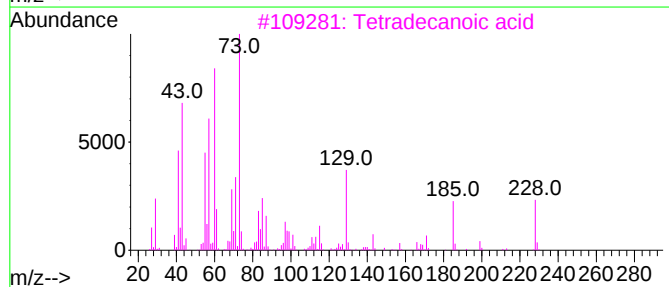
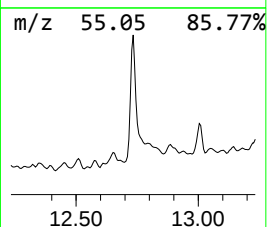
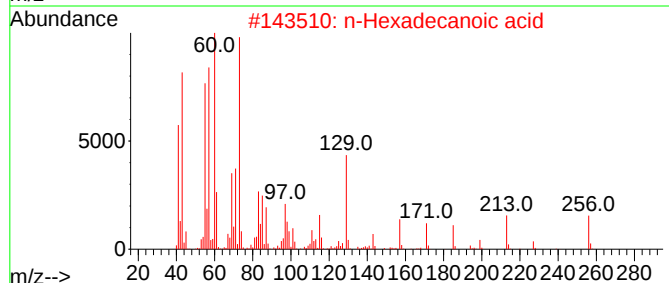
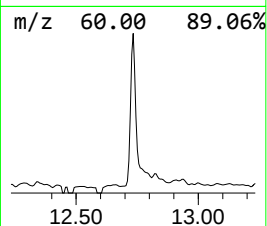
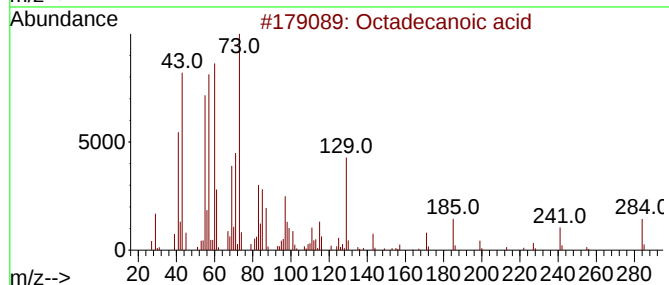
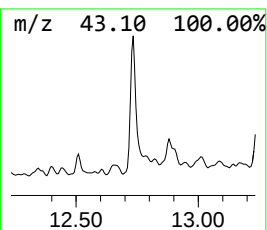
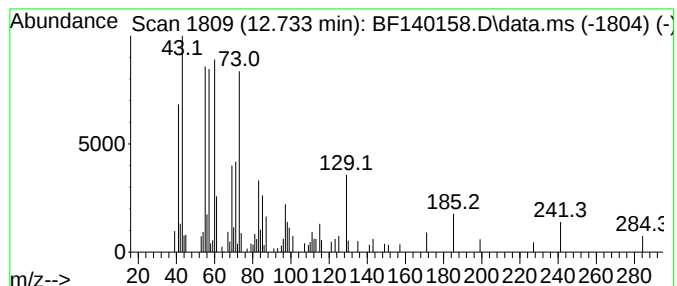
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	2.41 ng	99836	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	94
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			n-Decanoic acid	172	C10H20O2	000334-48-5	49
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	46



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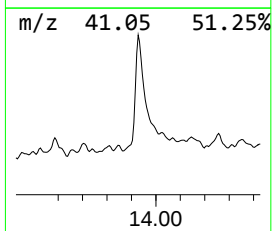
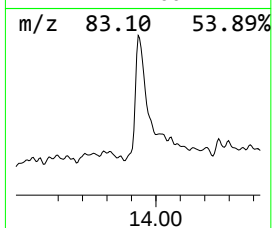
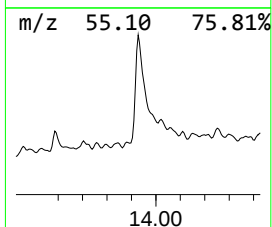
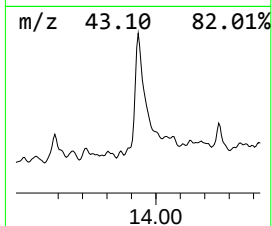
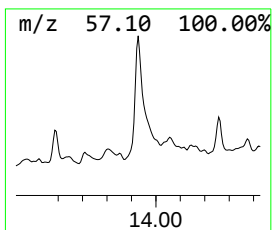
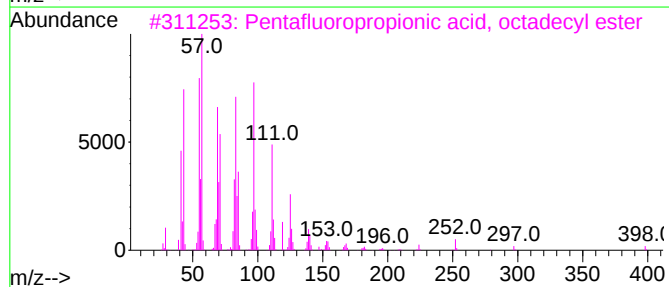
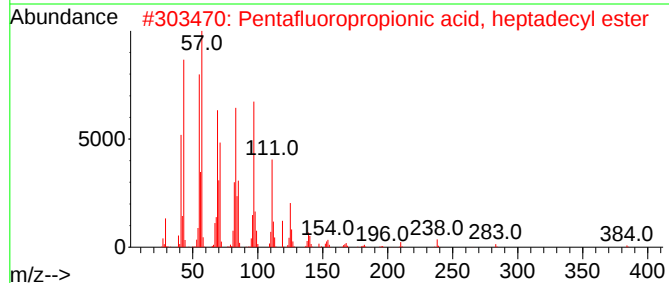
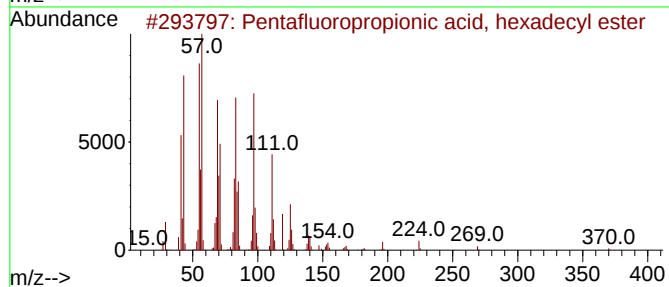
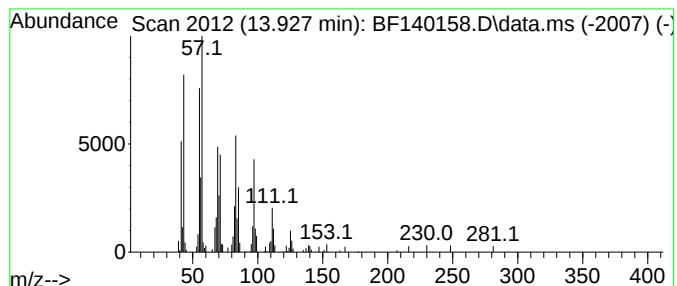
Instrument :
BNA_F
ClientSampleId :
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.927	6.75 ng	159313	Chrysene-d12	14.080	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hexadecyl	388	C19H33F5O2	006222-07-7	91
2	Pentafluoropropionic acid, heptadecyl	402	C20H35F5O2	959218-78-1	91
3	Pentafluoropropionic acid, octadecyl	416	C21H37F5O2	959261-25-7	91
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5	Heptafluorobutyric acid, hexadecyl	438	C20H33F7O2	006385-15-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103024\
Data File : BF140158.D
Acq On : 30 Oct 2024 15:34
Operator : RC/JU
Sample : P4611-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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...	2.163	61.3	ng	1844010	1	6.881	601354	20.0
2-Pentanone, 4-...	5.104	2.6	ng	79387	1	6.881	601354	20.0
Benzophenone	10.639	13.9	ng	596832	3	9.922	858587	20.0
n-Hexadecanoic ...	11.945	12.4	ng	512473	4	11.416	828947	20.0
Octadecanoic acid	12.733	2.4	ng	99836	4	11.416	828947	20.0
Pentafluoroprop...	13.927	6.8	ng	159313	5	14.080	472013	20.0