

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050125\
 Data File : BF142262.D
 Acq On : 01 May 2025 16:03
 Operator : RC/JU
 Sample : Q1903-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-4

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-BF043025.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142262.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.310	13	20	31	rVB2	48113	84325	2.00%	0.283%
2	5.128	485	499	509	rBV	299572	463208	11.00%	1.552%
3	5.516	559	565	570	rBV	2759385	3673370	87.21%	12.312%
4	6.522	729	736	741	rBV	2689572	3774423	89.61%	12.650%
5	6.904	796	801	806	rVB	984869	1215037	28.85%	4.072%
6	7.463	890	896	901	rBV	1827511	2326220	55.22%	7.797%
7	7.716	935	939	944	rVB	43527	50937	1.21%	0.171%
8	8.186	1014	1019	1024	rBV	1310606	1589218	37.73%	5.326%
9	9.263	1196	1202	1207	rBV	3329068	4212280	100.00%	14.118%
10	9.939	1312	1317	1322	rVB	1331621	1625671	38.59%	5.449%
11	10.651	1433	1438	1445	rBV	741076	926067	21.98%	3.104%
12	10.727	1445	1451	1462	rBV	1709180	2163633	51.36%	7.252%
13	10.963	1482	1491	1496	rBV	107658	138701	3.29%	0.465%
14	11.427	1565	1570	1575	rVB	1122335	1369851	32.52%	4.591%
15	11.951	1654	1659	1663	rBV	86943	127215	3.02%	0.426%
16	12.457	1739	1745	1753	rBV2	30939	62940	1.49%	0.211%
17	13.016	1834	1840	1845	rBV	2508185	3231757	76.72%	10.832%
18	13.910	1987	1992	2005	rBV	91805	159462	3.79%	0.534%
19	14.068	2012	2019	2031	rBV	912490	1246636	29.60%	4.178%
20	14.839	2145	2150	2164	rBV3	97234	226927	5.39%	0.761%
21	15.557	2266	2272	2278	rBV	761860	1168458	27.74%	3.916%

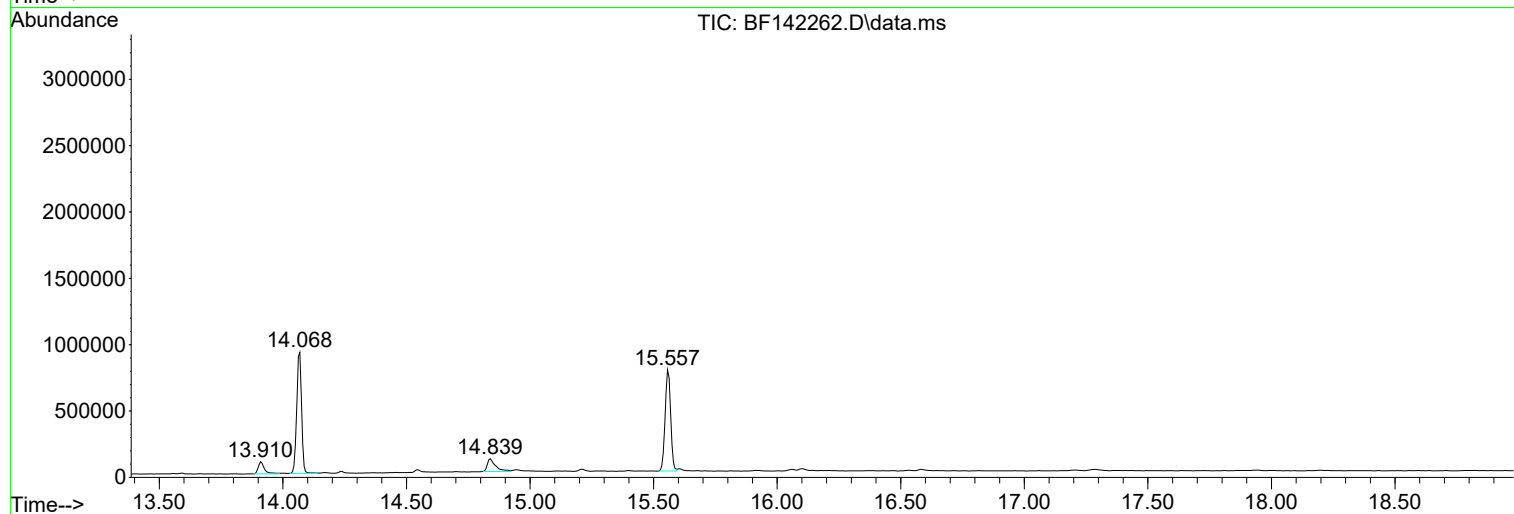
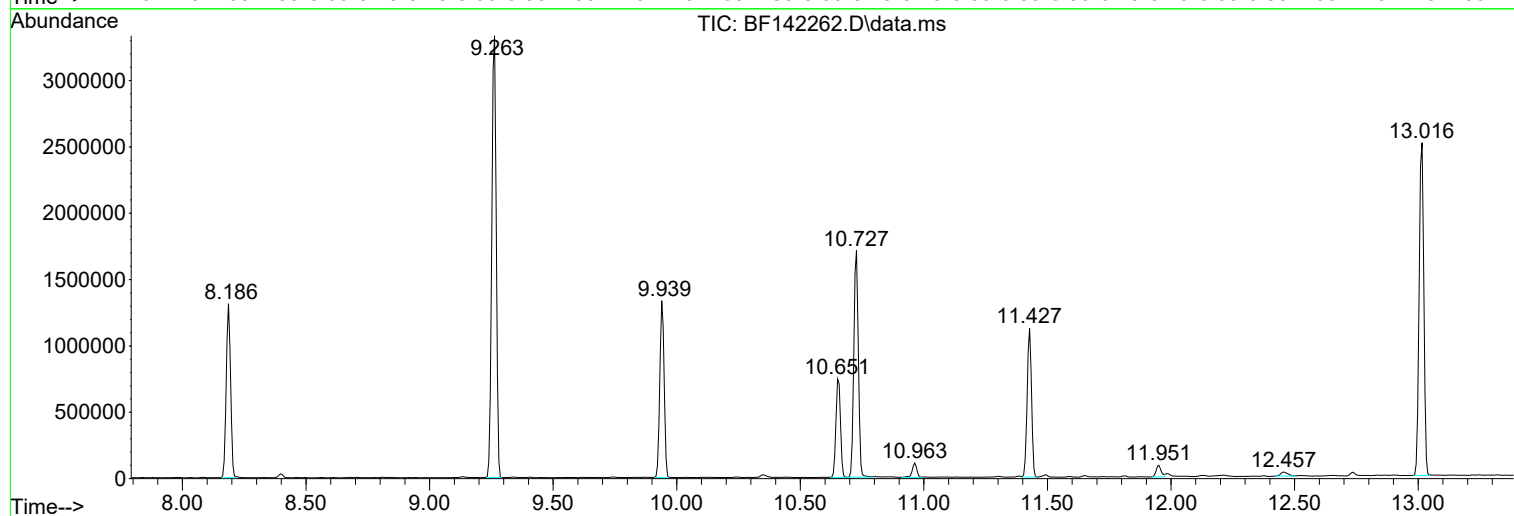
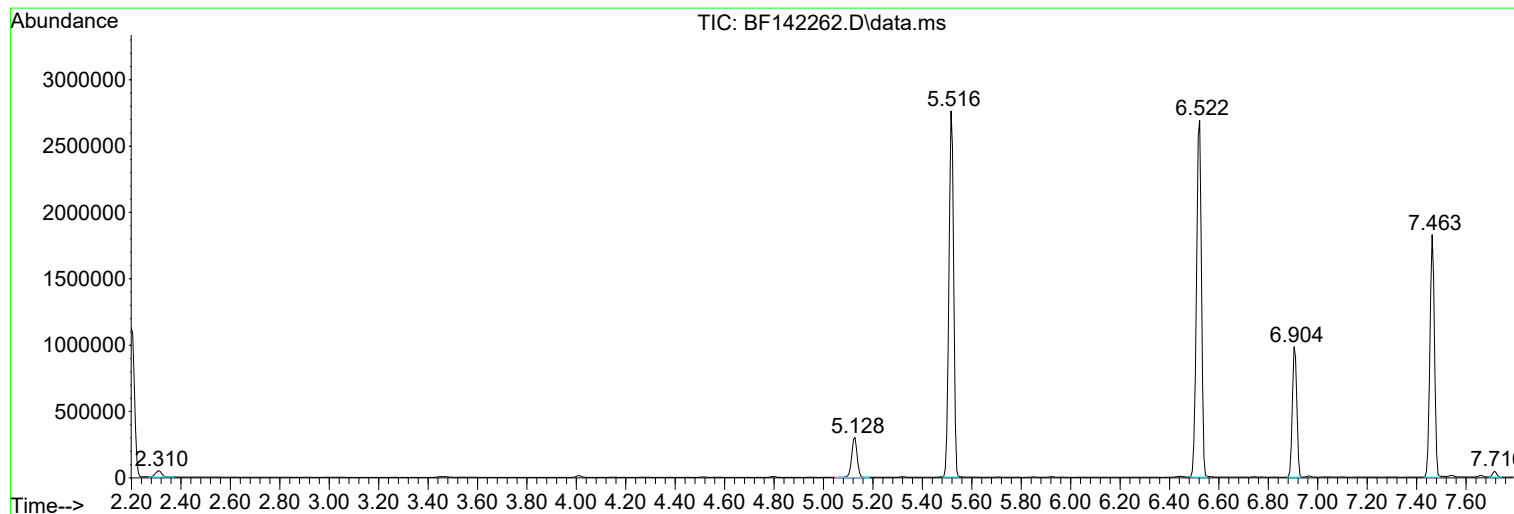
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF142262.D
Acq On : 01 May 2025 16:03
Operator : RC/JU
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Instrument :
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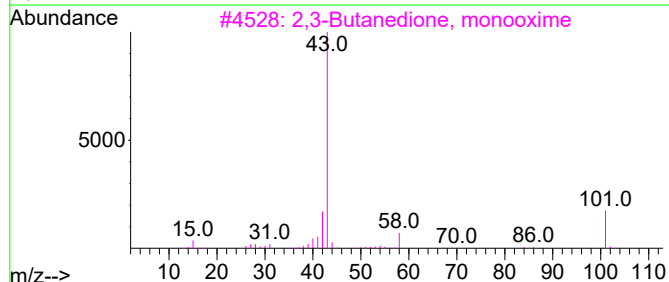
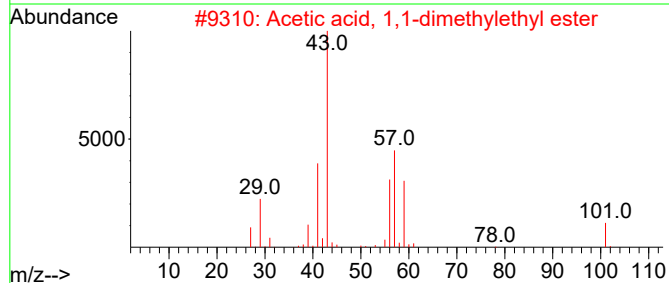
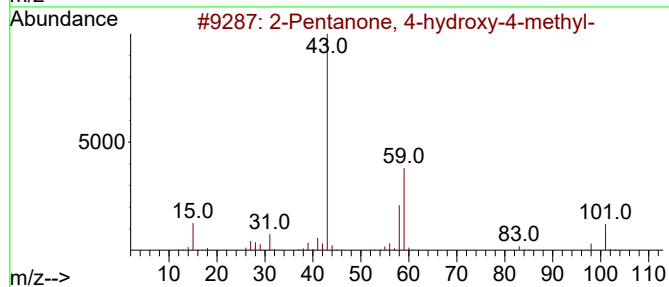
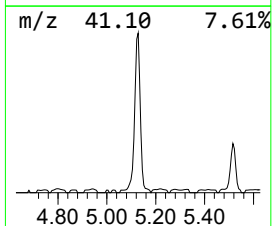
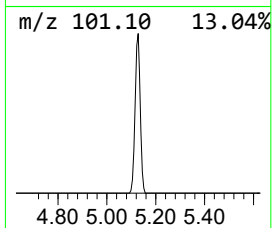
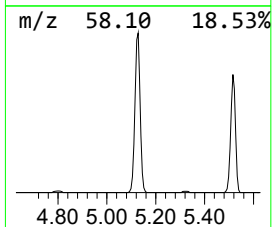
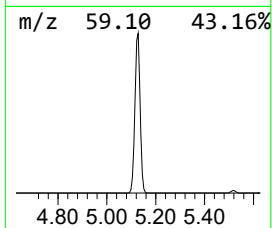
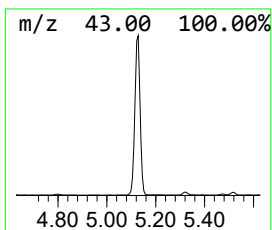
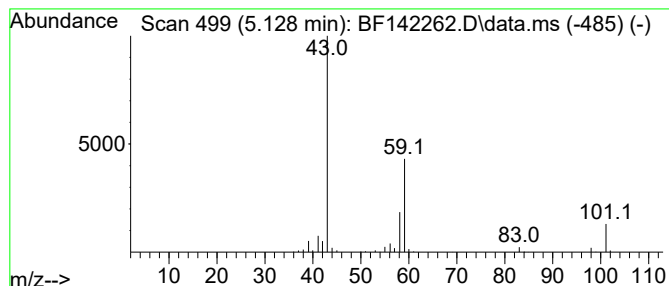
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	7.62 ng	463208	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	Acetone	58	C3H6O	000067-64-1	12		



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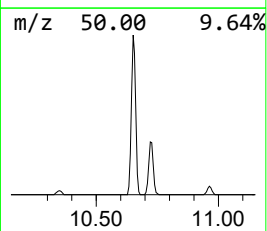
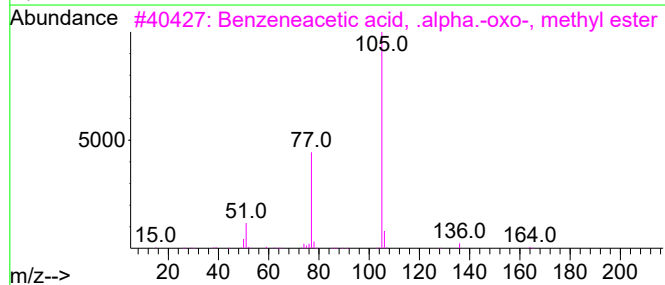
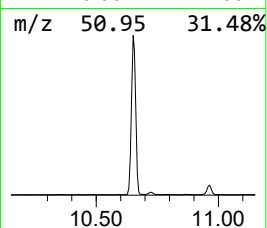
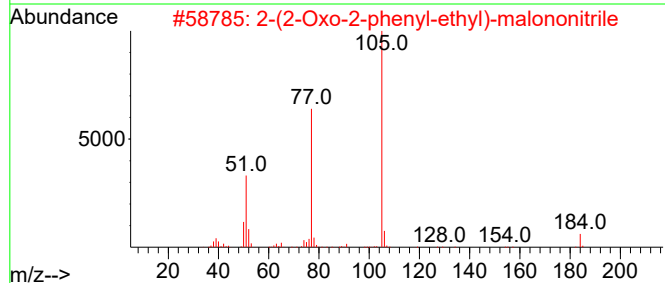
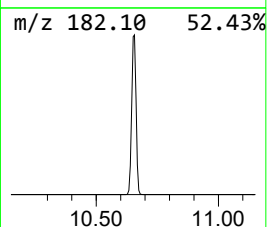
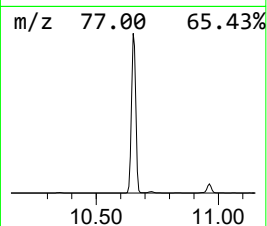
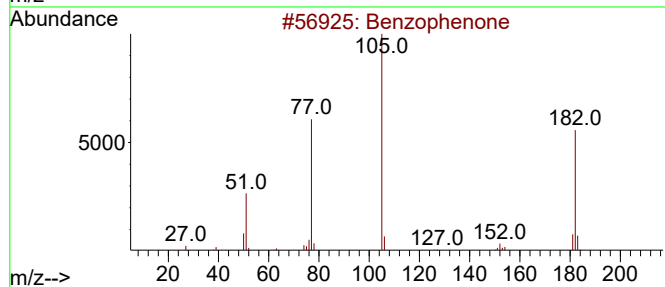
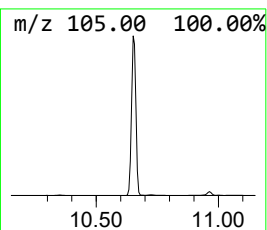
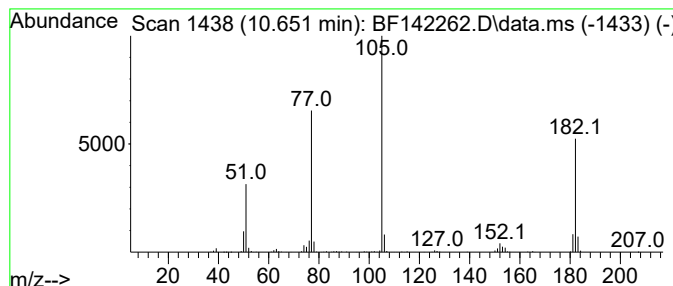
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	11.39 ng	926067	Acenaphthene-d10	9.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	58
3			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	52
4			Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	50
5			Vinyl benzoate	148	C9H8O2	000769-78-8	50



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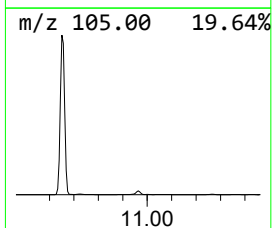
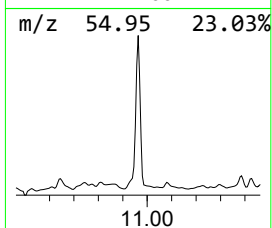
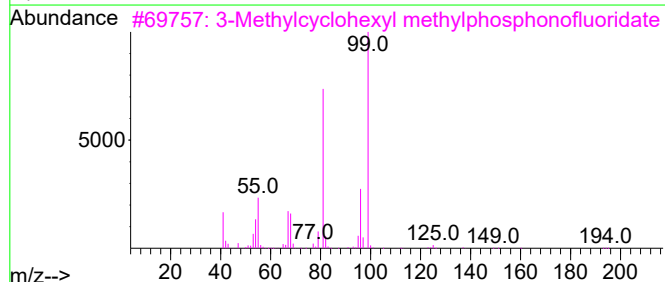
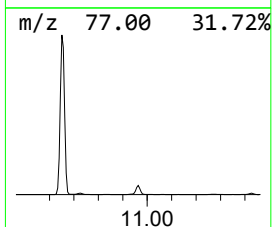
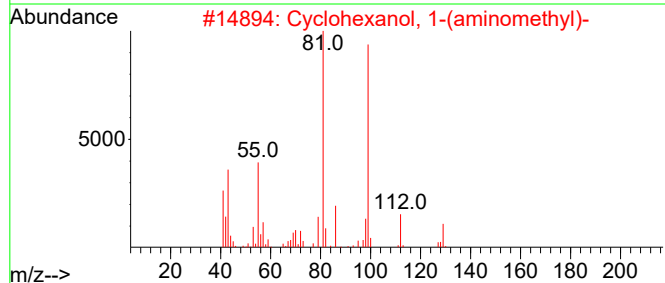
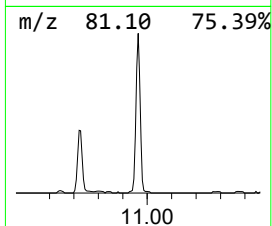
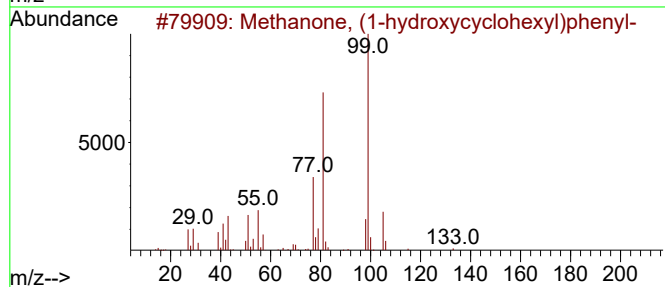
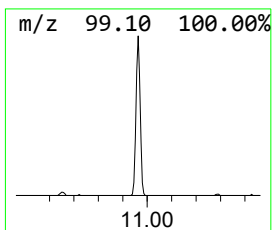
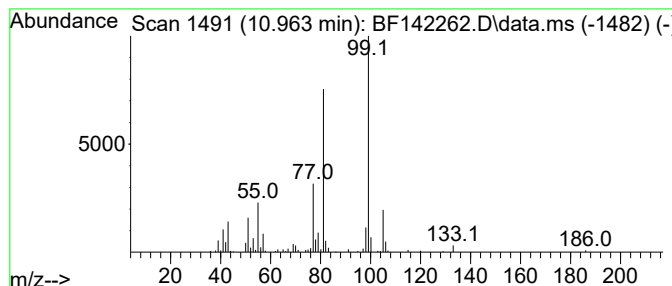
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Methanone, (1-hydroxycyclohexyl) Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.963	2.03 ng	138701	Phenanthrene-d10	11.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	91
2			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	45
3			3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	42
4			2-Methylcyclosarin	194	C8H16FO2P	085473-32-1	40
5			Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	36



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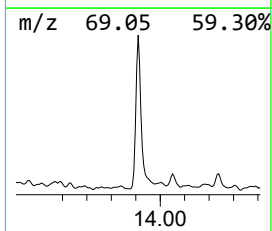
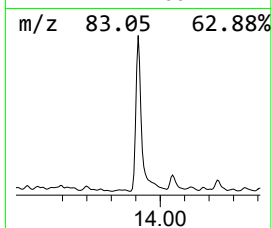
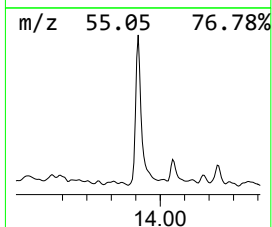
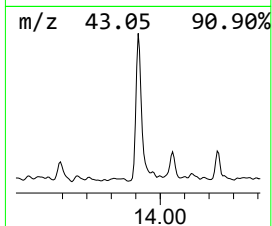
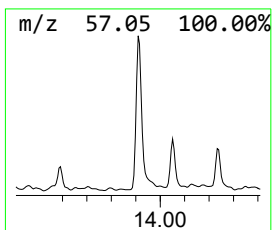
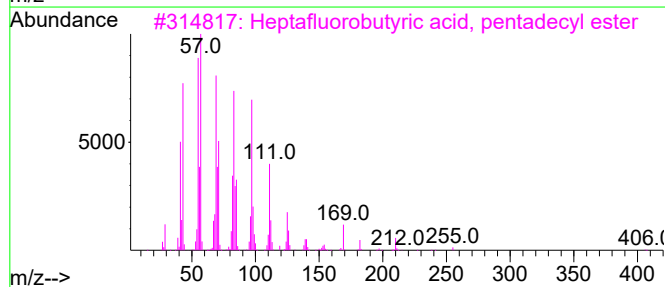
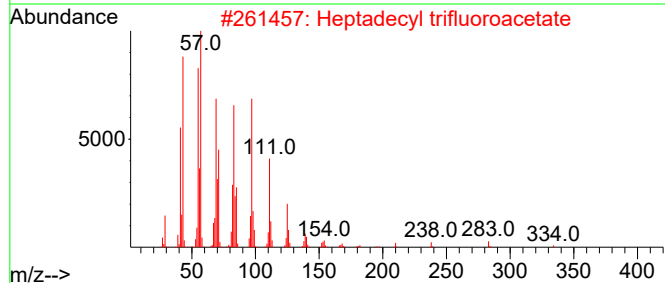
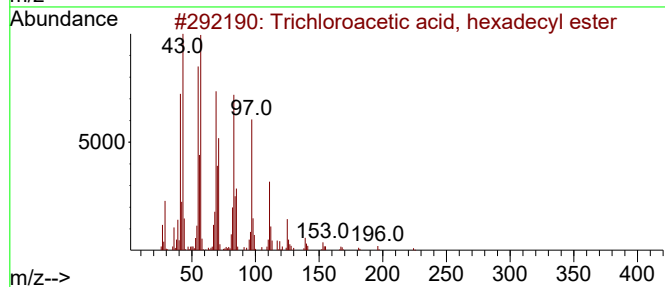
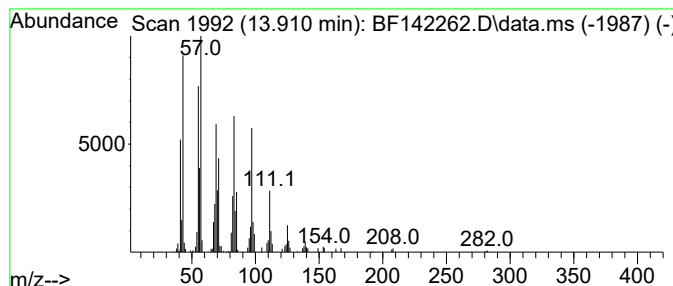
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	2.56 ng	159462	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5			1-Hexacosene	364	C26H52	018835-33-1	94



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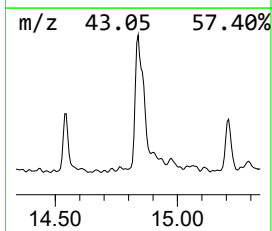
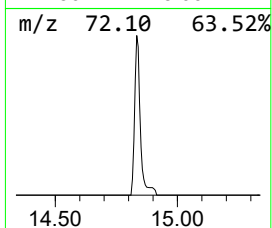
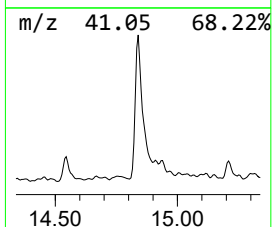
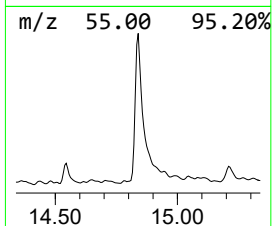
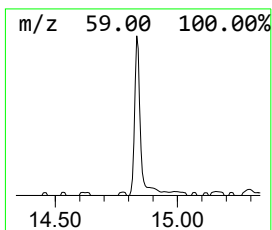
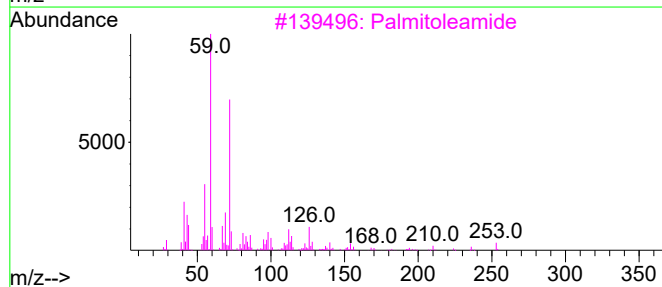
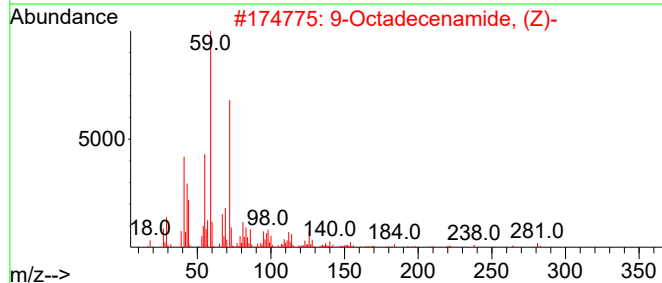
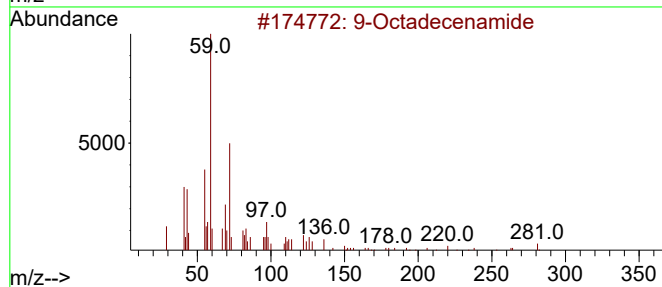
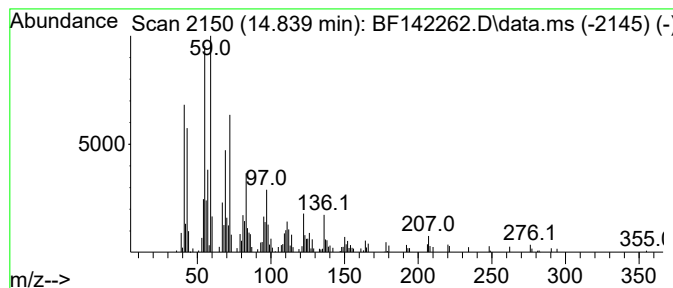
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenamide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	3.88 ng	226927	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide	281	C18H35NO	003322-62-1	72
2			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	70
3			Palmitoleamide	253	C16H31NO	106010-22-4	62
4			13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	58
5			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	47



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.128	7.6	ng	463208	1	6.904	1215040	20.0
Benzophenone	10.651	11.4	ng	926067	3	9.939	1625670	20.0
Methanone, (1-h...	10.963	2.0	ng	138701	4	11.427	1369850	20.0
Trichloroacetic...	13.910	2.6	ng	159462	5	14.068	1246640	20.0
9-Octadecenamide	14.839	3.9	ng	226927	6	15.557	1168460	20.0