

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080723\
 Data File : BF134644.D
 Acq On : 07 Aug 2023 09:48
 Operator : CG\JU
 Sample : 03891-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1

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-BF080123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134644.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	14	19	25	rBV	82310	108544	1.97%	0.265%
2	2.299	30	36	42	rVB	1496593	2009346	36.44%	4.900%
3	2.375	42	49	56	rBV	45848	117391	2.13%	0.286%
4	5.046	499	503	511	rVB	133069	180065	3.27%	0.439%
5	5.434	563	569	572	rBV	4705344	4947879	89.73%	12.065%
6	6.434	733	739	742	rBV	4376554	5070080	91.95%	12.363%
7	6.628	769	772	777	rBV	166446	146739	2.66%	0.358%
8	6.798	797	801	804	rBV	1524192	1175489	21.32%	2.866%
9	7.357	890	896	899	rBV	3143962	3324132	60.29%	8.106%
10	8.075	1013	1018	1021	rBV	1945497	1581992	28.69%	3.858%
11	9.157	1196	1202	1205	rBV	5658978	5513940	100.00%	13.445%
12	9.269	1218	1221	1225	rVB	93057	82506	1.50%	0.201%
13	9.828	1311	1316	1320	rBV	1918317	1740864	31.57%	4.245%
14	10.186	1362	1377	1378	rBV2	111095	410213	7.44%	1.000%
15	10.622	1446	1451	1454	rBV	3670046	3502479	63.52%	8.540%
16	10.745	1469	1472	1478	rBV2	36511	57630	1.05%	0.141%
17	11.322	1566	1570	1573	rBV	1814928	1672297	30.33%	4.078%
18	11.386	1579	1581	1584	rVB3	77084	66611	1.21%	0.162%
19	11.863	1656	1662	1670	rBV	814145	973933	17.66%	2.375%
20	12.645	1792	1795	1802	rBV2	252287	271330	4.92%	0.662%
21	12.922	1837	1842	1845	rBV	5045845	5198381	94.28%	12.676%
22	13.821	1992	1995	2005	rVB	456005	512770	9.30%	1.250%
23	13.963	2015	2019	2023	rBV	1199137	1173213	21.28%	2.861%
24	14.457	2101	2103	2111	rVB2	67465	78200	1.42%	0.191%
25	14.763	2152	2155	2160	rVB	50654	60746	1.10%	0.148%
26	15.104	2211	2213	2218	rVB2	53464	56103	1.02%	0.137%
27	15.433	2264	2269	2276	rBV	825190	977542	17.73%	2.384%

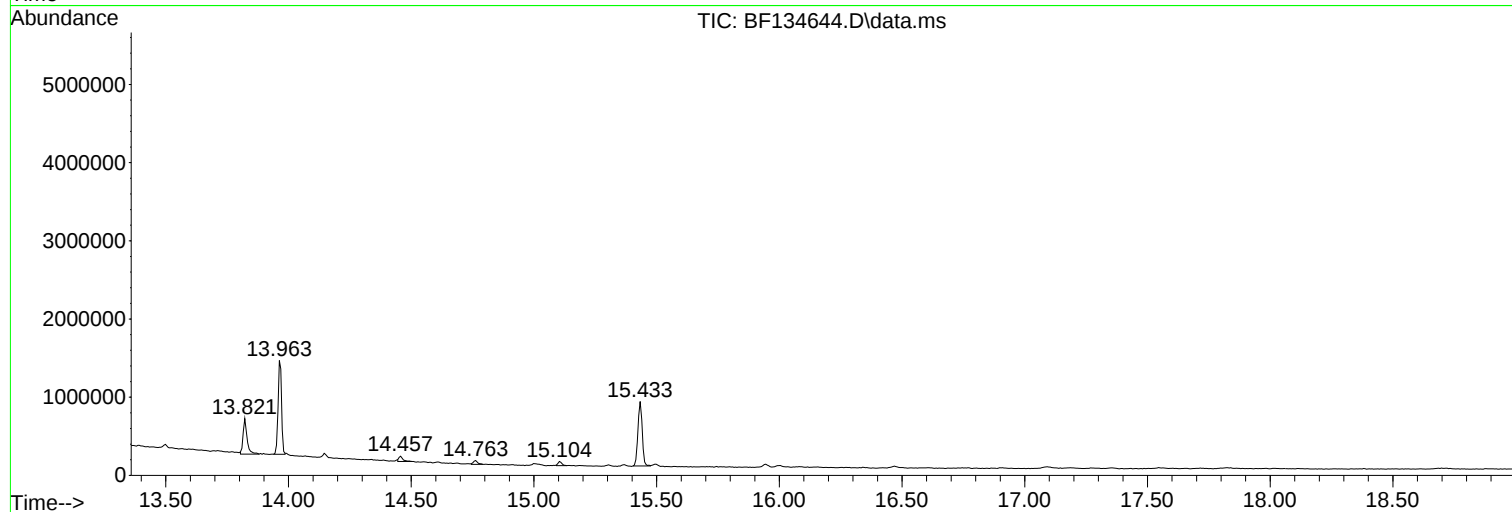
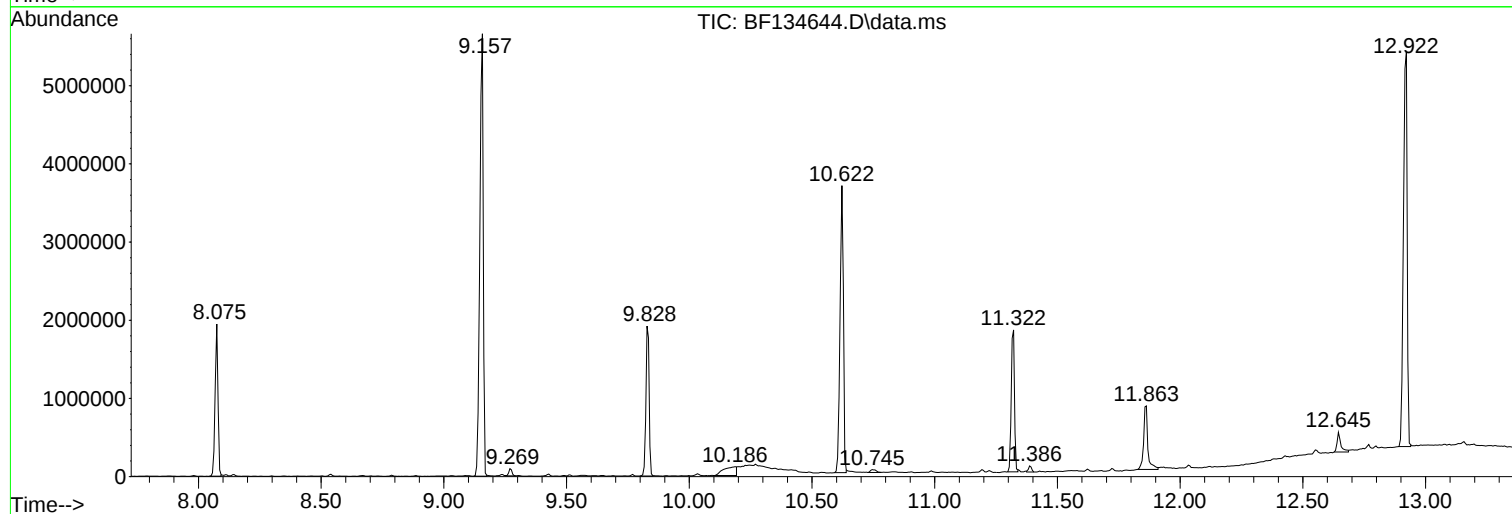
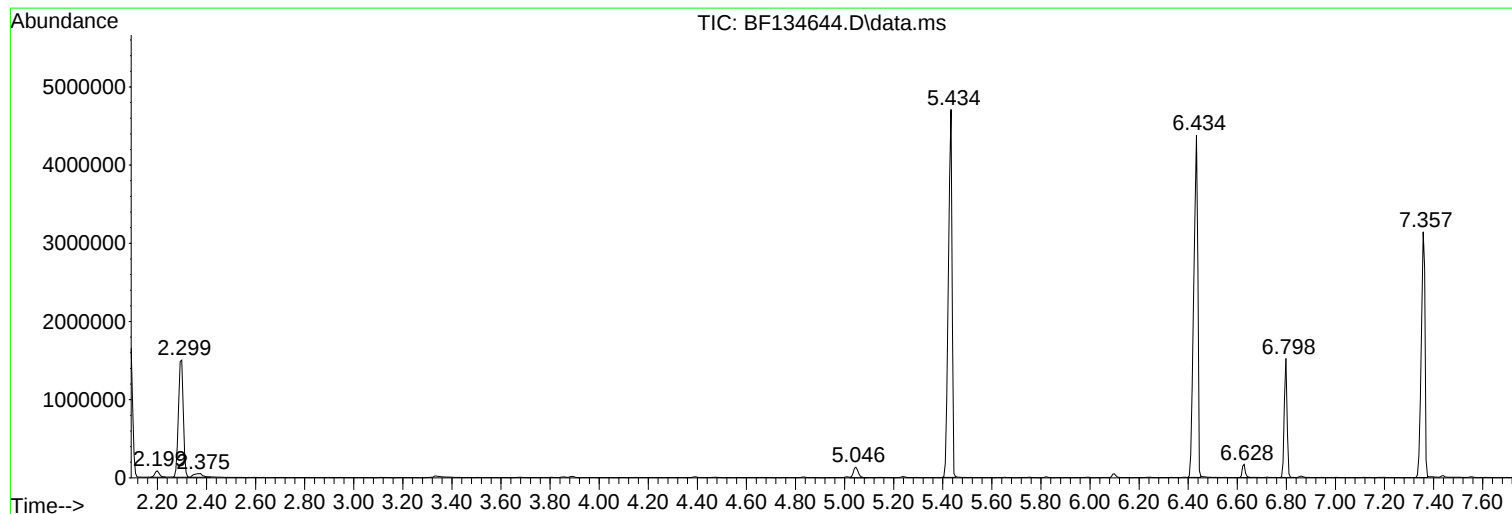
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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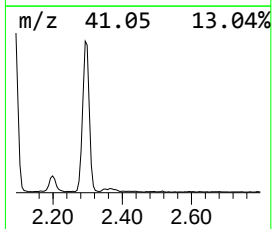
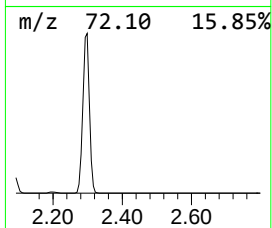
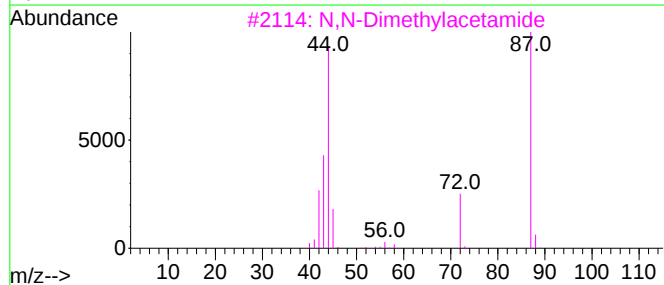
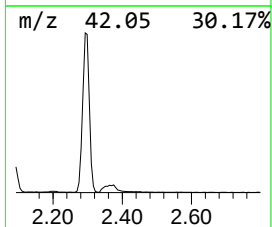
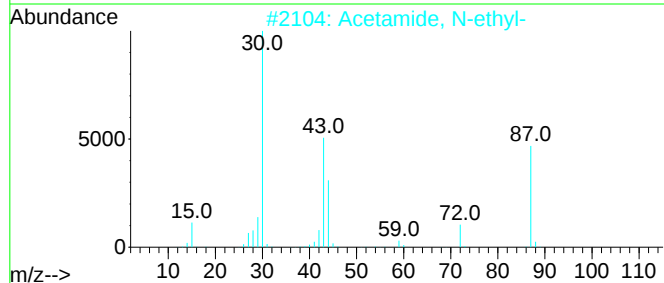
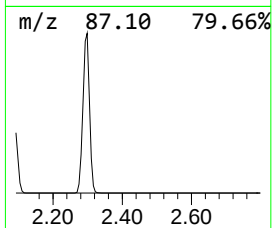
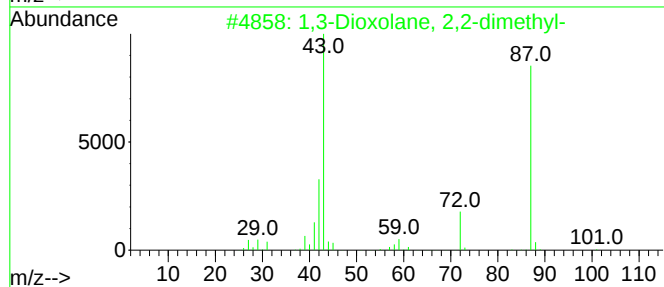
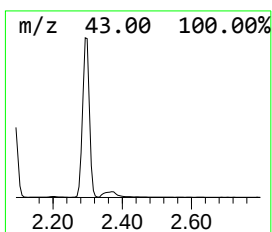
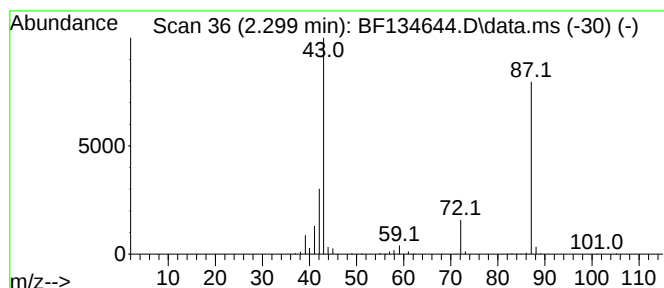
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3-Dioxolane, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.299	34.19 ng	2009350	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2,2-dimethyl-	102	C5H10O2	002916-31-6	90
2			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	72
3			N,N-Dimethylacetamide	87	C4H9NO	000127-19-5	59
4			2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	50
5			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	42



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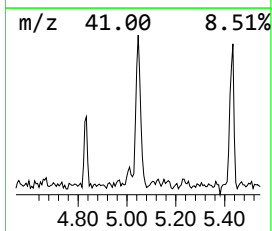
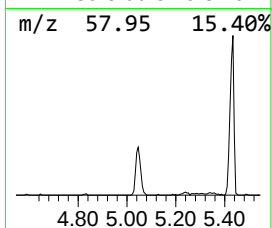
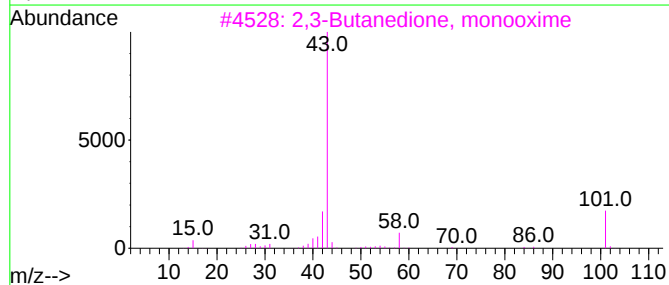
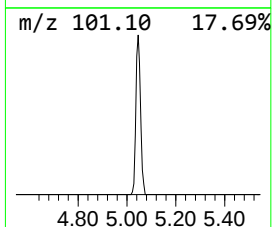
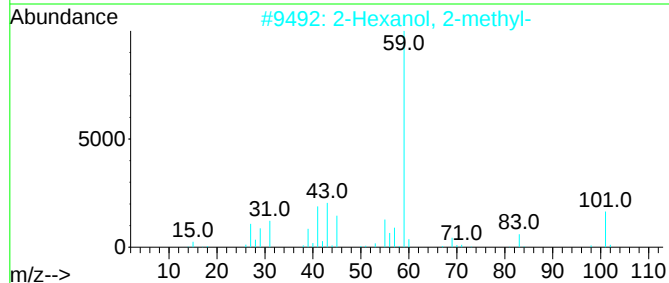
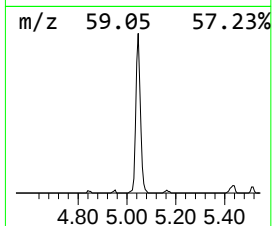
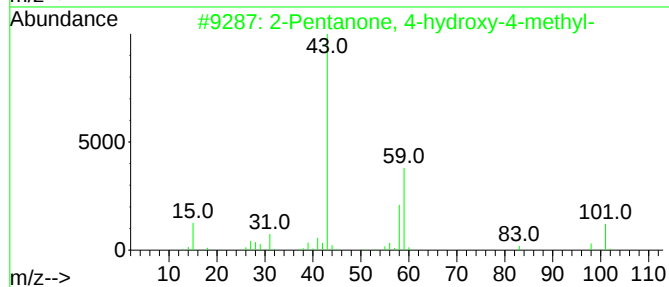
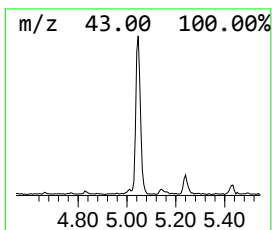
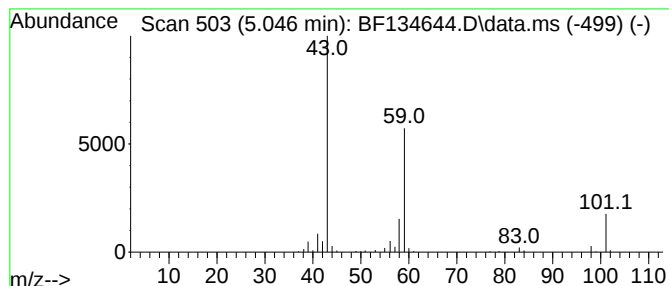
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.046	3.06 ng	180065	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27		
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		



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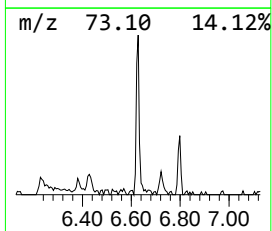
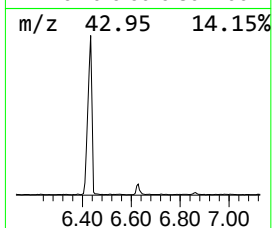
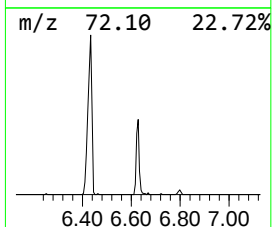
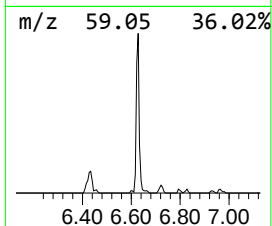
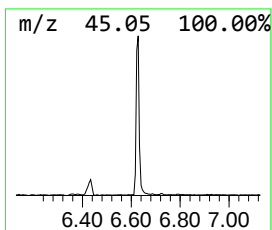
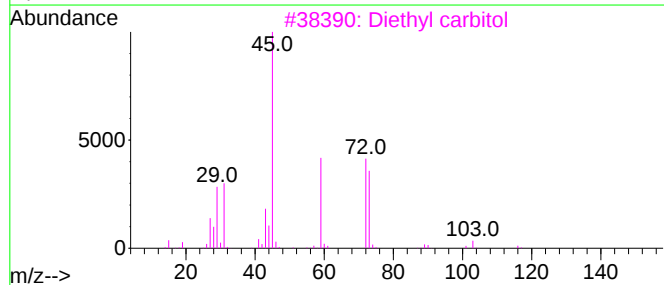
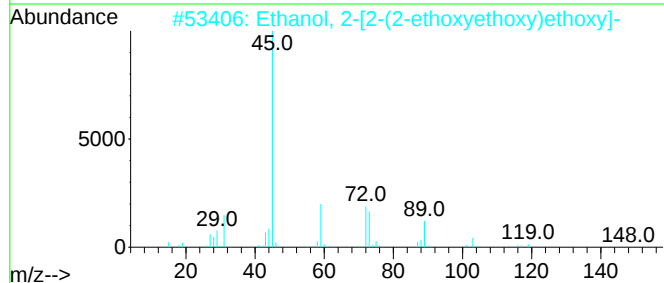
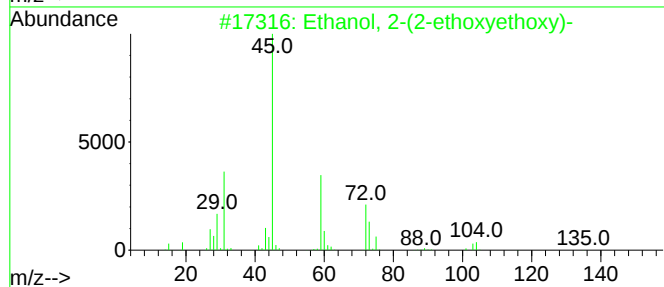
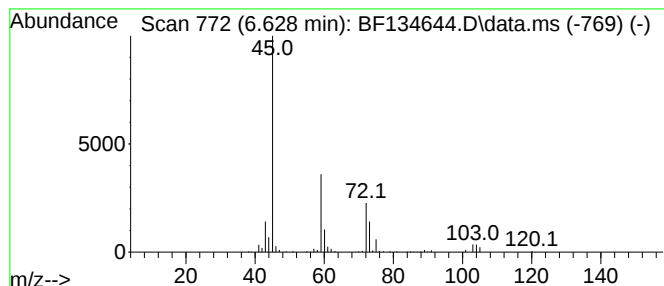
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.628	2.50 ng	146739	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	72
3			Diethyl carbitol	162	C8H18O3	000112-36-7	72
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
5			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	43



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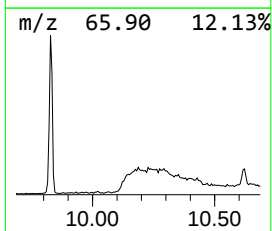
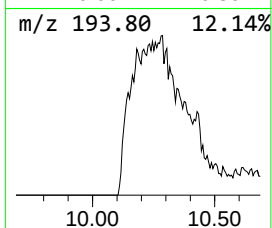
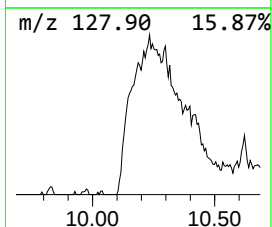
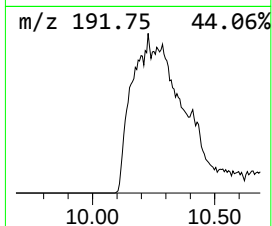
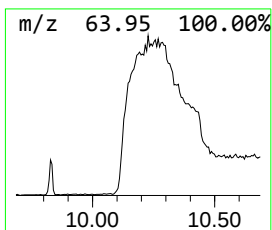
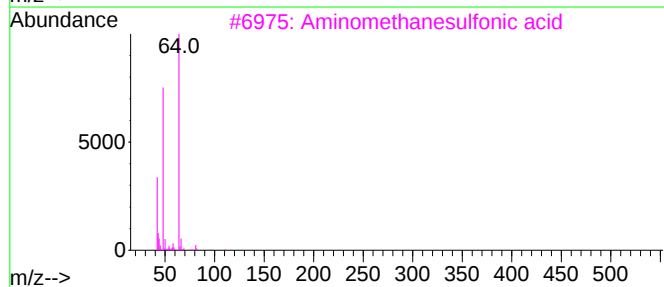
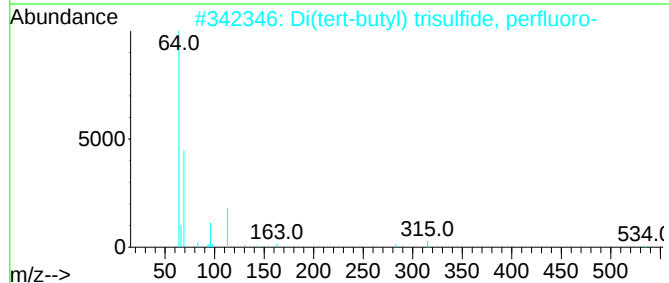
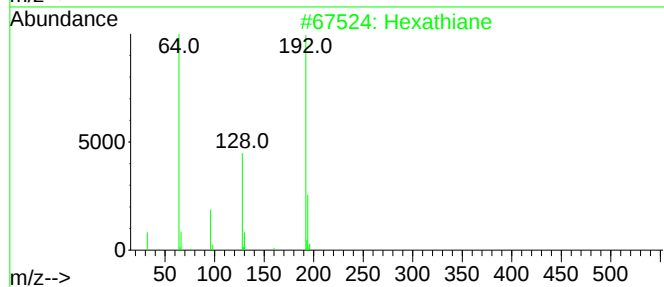
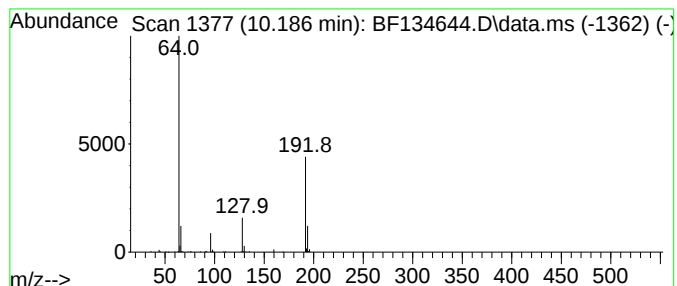
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Peak Number 4 Hexathiane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.186	4.71 ng	410213	Acenaphthene-d10	9.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexathiane	192	S6	013798-23-7	91
2			Di(tert-butyl) trisulfide, perfluoro-	534	C8F18S3	016005-64-4	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	5
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	5
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	5



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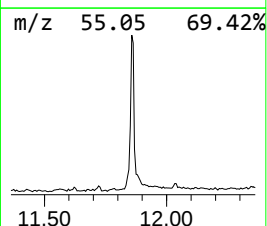
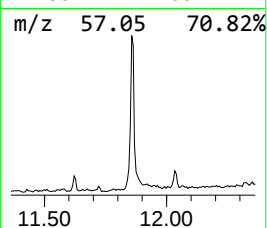
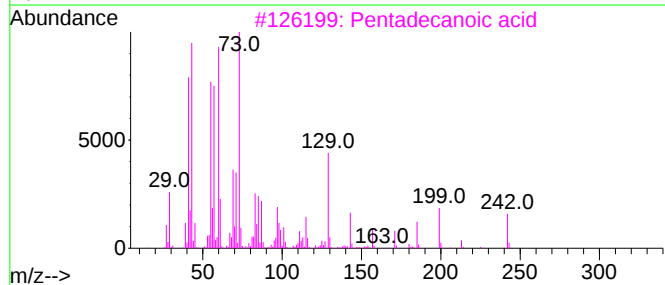
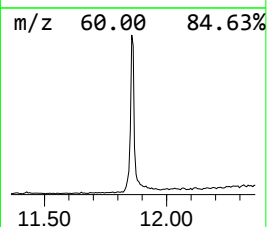
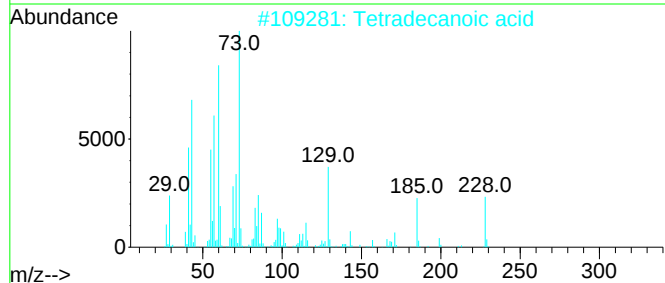
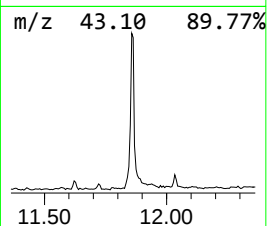
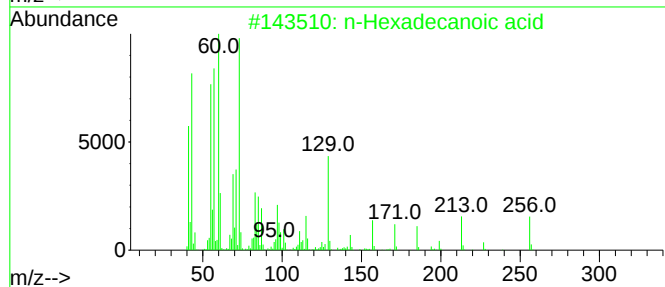
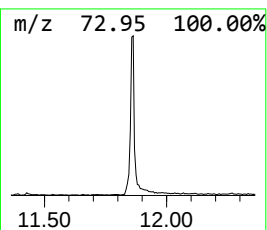
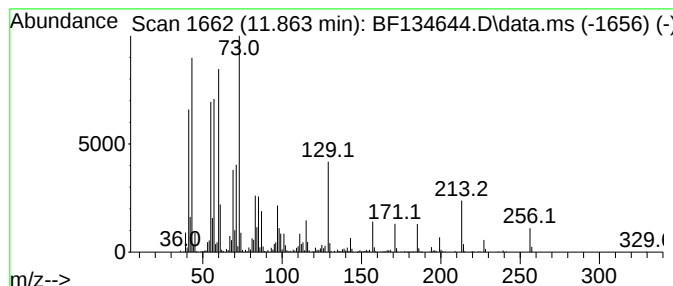
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	11.65 ng	973933	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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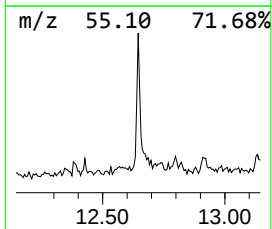
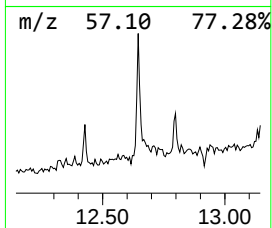
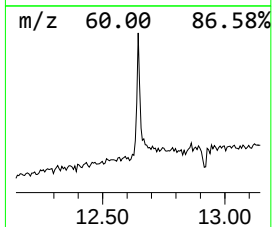
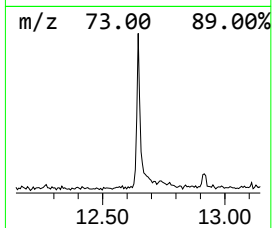
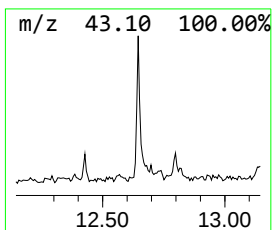
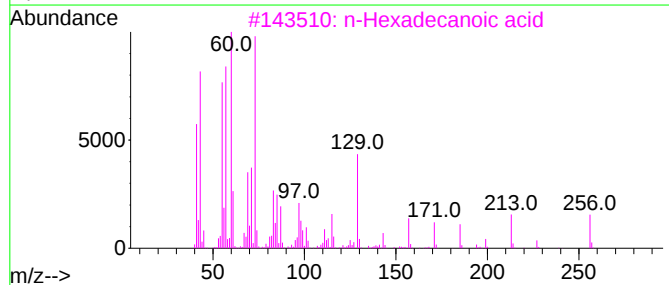
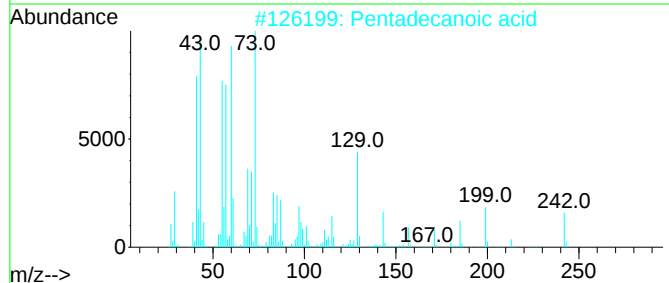
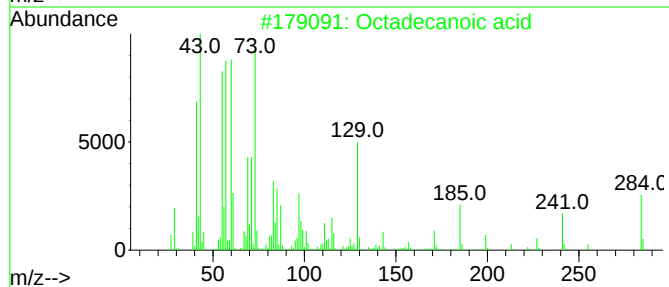
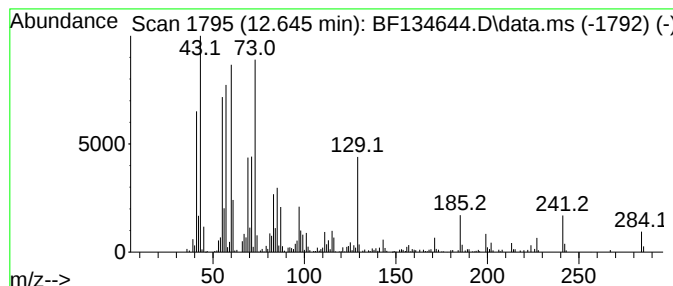
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	4.63 ng	271330	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080723\
Data File : BF134644.D
Acq On : 07 Aug 2023 09:48
Operator : CG\JU
Sample : 03891-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

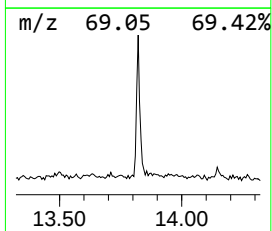
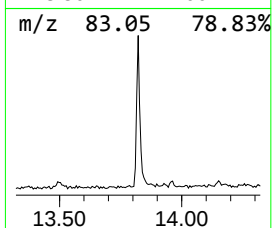
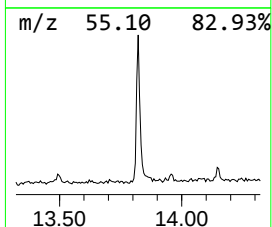
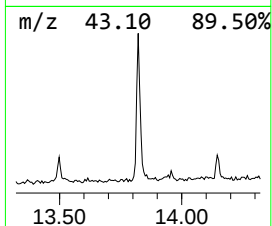
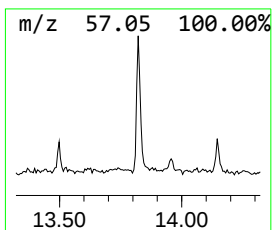
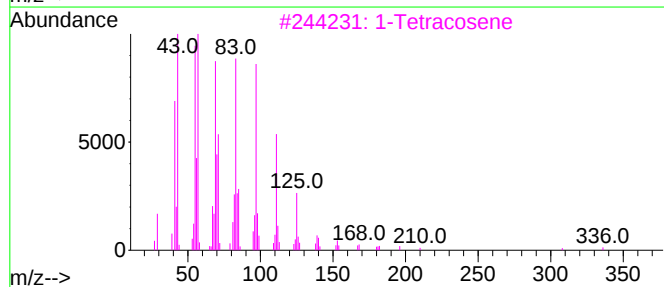
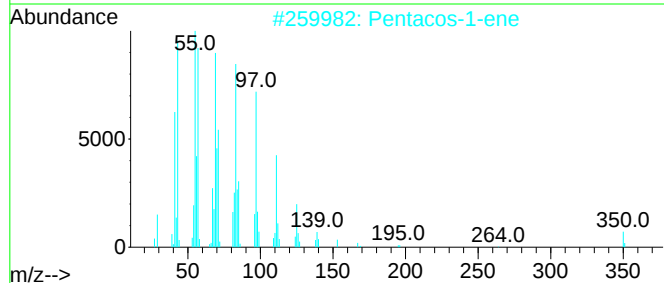
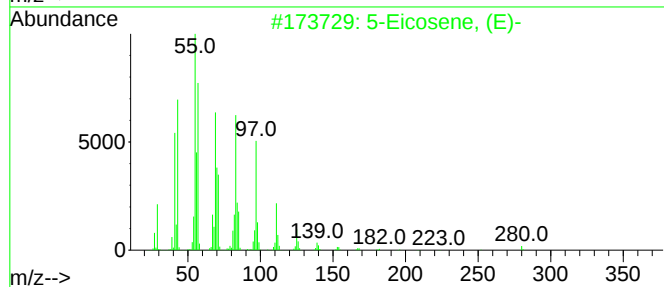
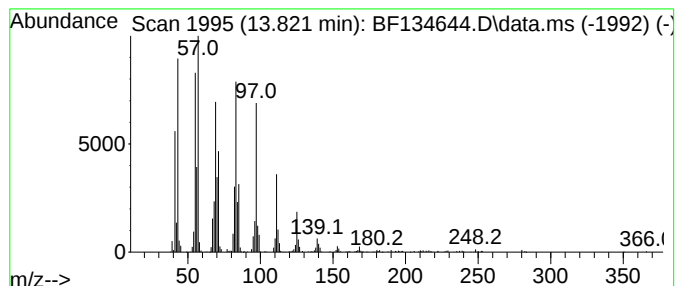
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.822	8.74 ng	512770	Chrysene-d12	13.963

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2		Pentacos-1-ene	350	C25H50	016980-85-1	94
3		1-Tetracosene	336	C24H48	010192-32-2	94
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080723\
Data File : BF134644.D
Acq On : 07 Aug 2023 09:48
Operator : CG\JU
Sample : 03891-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF080123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3-Dioxolane, ...	2.299	34.2	ng	2009350	1	6.798	1175490	20.0
2-Pentanone, 4-...	5.046	3.1	ng	180065	1	6.798	1175490	20.0
Ethanol, 2-(2-e...	6.628	2.5	ng	146739	1	6.798	1175490	20.0
Hexathiane	10.186	4.7	ng	410213	3	9.828	1740860	20.0
n-Hexadecanoic ...	11.863	11.7	ng	973933	4	11.322	1672300	20.0
Octadecanoic acid	12.645	4.6	ng	271330	5	13.963	1173210	20.0
5-Eicosene, (E)-	13.822	8.7	ng	512770	5	13.963	1173210	20.0