

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092520\
 Data File : BF121697.D
 Acq On : 25 Sep 2020 15:53
 Operator : JU/CG
 Sample : L4102-08
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-2B-(3.0-3.5)

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF091020.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	9	13	22	rVB	56727	87913	2.42%	0.410%
2	5.010	493	497	508	rVB	89491	117252	3.23%	0.547%
3	5.416	561	566	569	rBV	3105888	2796168	77.11%	13.044%
4	6.434	734	739	742	rBV	3018668	2863471	78.96%	13.358%
5	6.628	769	772	785	rBV	232250	226088	6.23%	1.055%
6	6.792	797	800	804	rBV	550754	480203	13.24%	2.240%
7	7.363	891	897	900	rBV	1984144	2044763	56.39%	9.539%
8	8.081	1015	1019	1027	rBV	741278	636180	17.54%	2.968%
9	9.157	1197	1202	1205	rBV	3894768	3626323	100.00%	16.916%
10	9.551	1265	1269	1272	rBV	678955	560631	15.46%	2.615%
11	9.592	1272	1276	1279	rVV2	145645	160244	4.42%	0.748%
12	9.651	1283	1286	1289	rBV	131144	107533	2.97%	0.502%
13	9.704	1291	1295	1299	rBV5	62720	128553	3.54%	0.600%
14	9.833	1311	1317	1321	rBV2	1012805	1144861	31.57%	5.341%
15	10.627	1448	1452	1455	rBV	1932776	2122864	58.54%	9.903%
16	12.927	1840	1843	1846	rVB	2701905	2563626	70.69%	11.959%
17	13.974	2018	2021	2023	rVB	529270	531745	14.66%	2.481%
18	14.998	2192	2195	2198	rBV	86804	100699	2.78%	0.470%
19	15.351	2252	2255	2261	rVB	87327	111581	3.08%	0.521%
20	15.415	2261	2266	2269	rBV	385363	482204	13.30%	2.249%
21	15.868	2339	2343	2348	rVB	63622	93292	2.57%	0.435%
22	15.933	2349	2354	2361	rBV6	52696	134802	3.72%	0.629%
23	16.839	2503	2508	2514	rVB2	36323	69834	1.93%	0.326%
24	17.268	2576	2581	2589	rVB	39600	81315	2.24%	0.379%
25	18.692	2816	2823	2833	rVB3	59754	164486	4.54%	0.767%

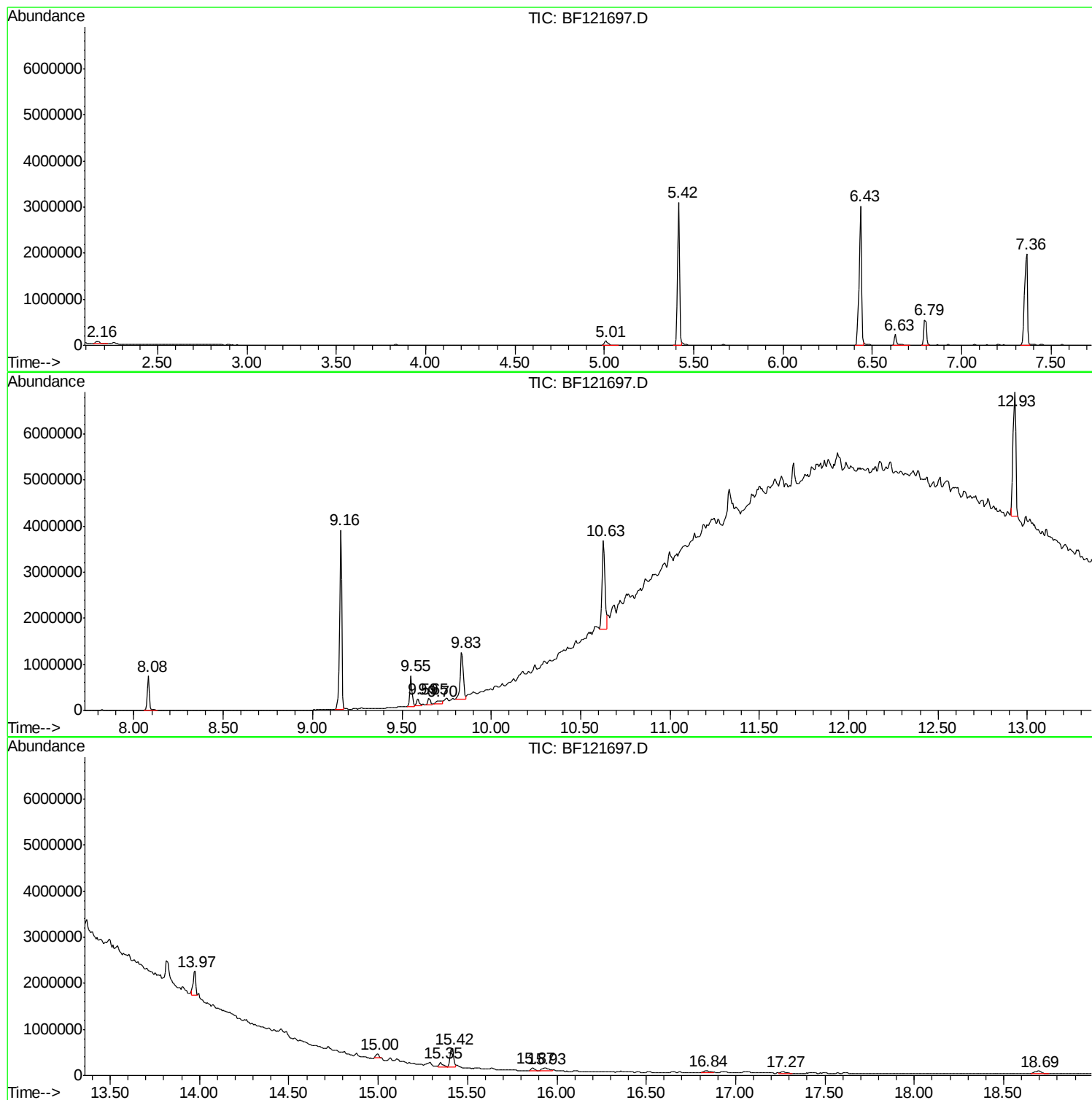
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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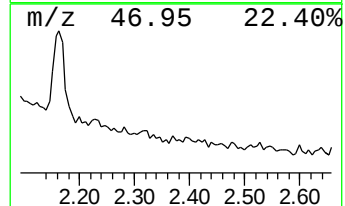
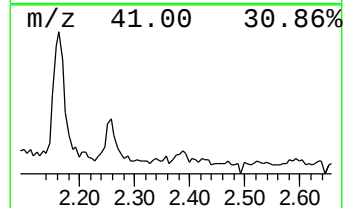
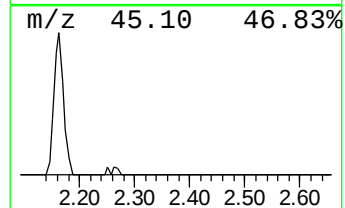
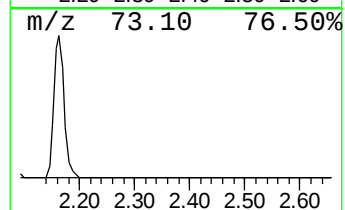
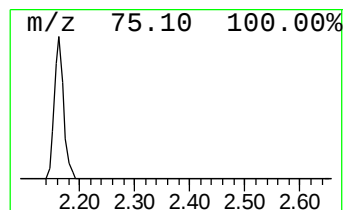
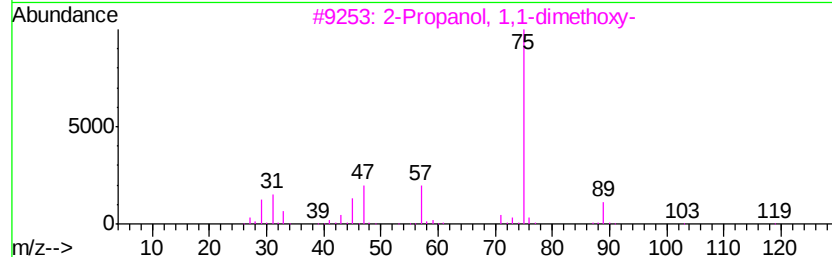
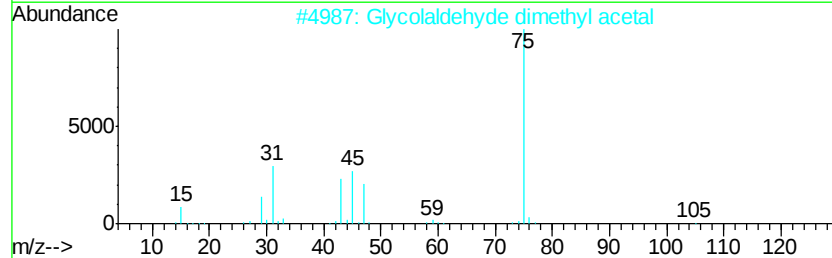
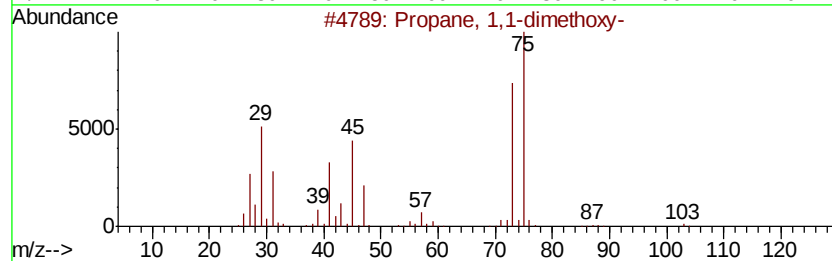
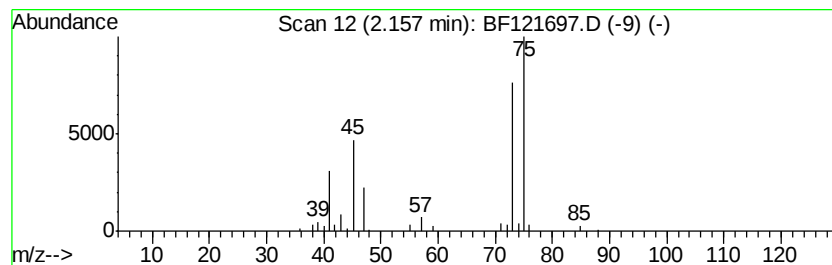
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	3.66 ng	87913	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	72
2		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	45
3		2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	36
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
5		Silane, methylenebis-	76	CH8Si2	001759-88-2	9



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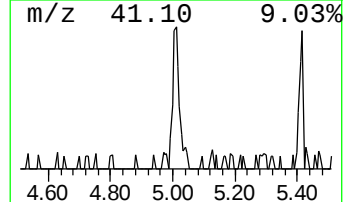
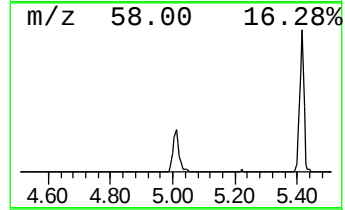
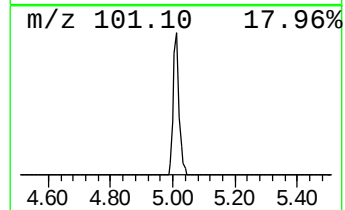
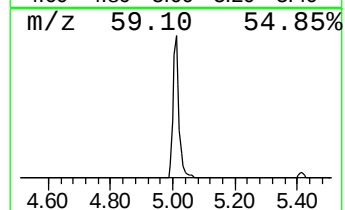
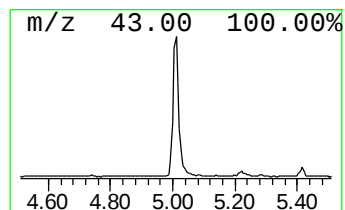
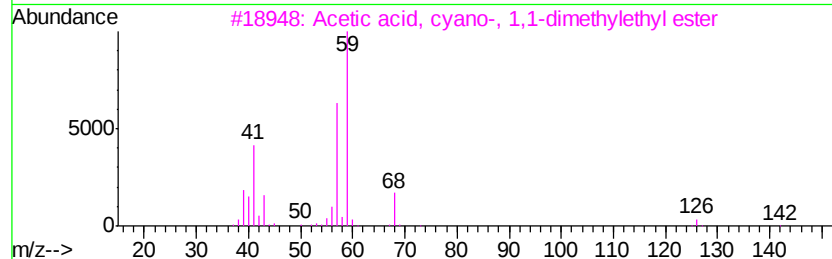
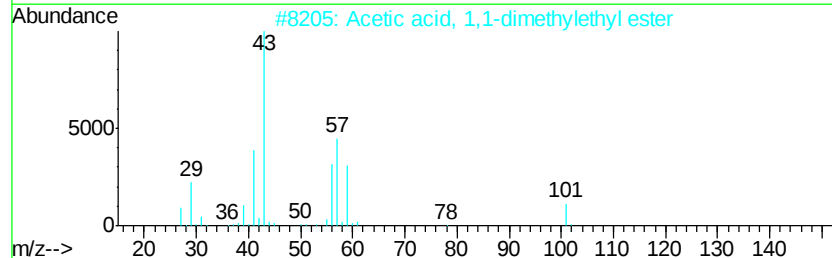
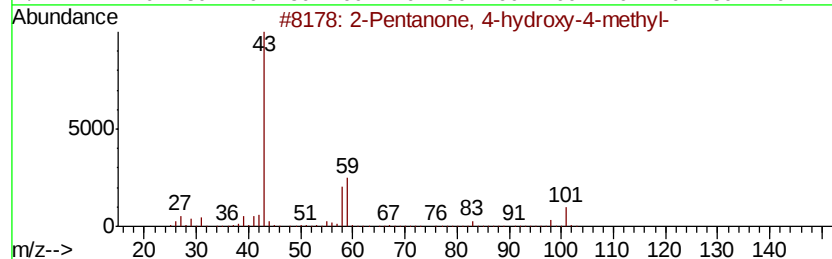
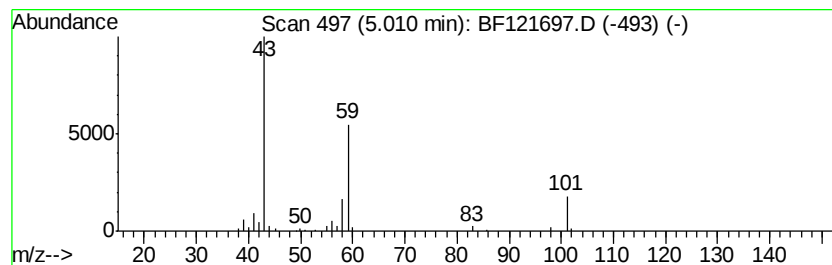
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.01	4.88 ng	117252	1,4-Dichlorobenzene-d4	6.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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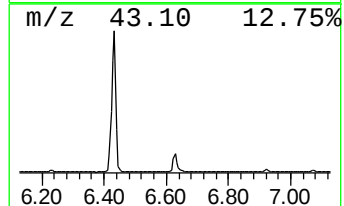
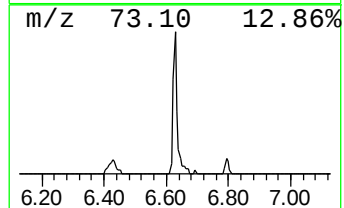
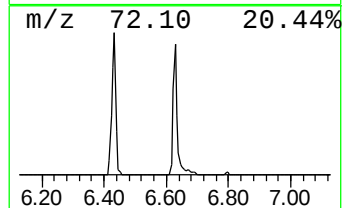
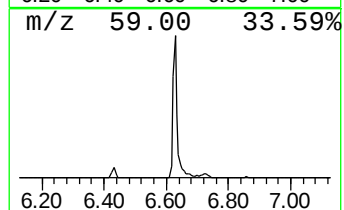
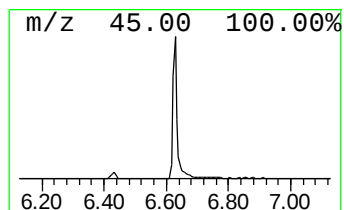
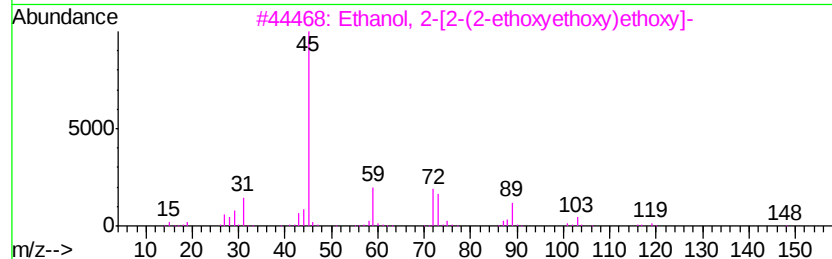
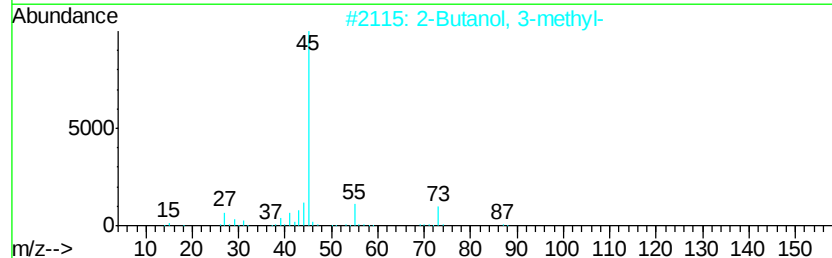
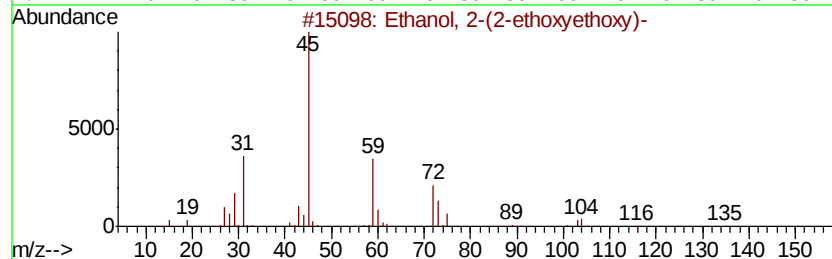
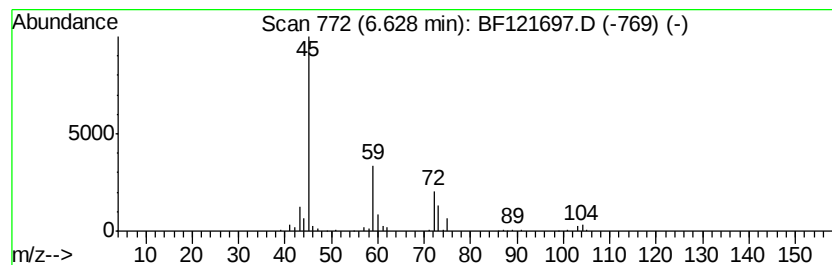
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	9.42 ng	226088	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2		2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	47
3		Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	38
4		2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
5		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	37



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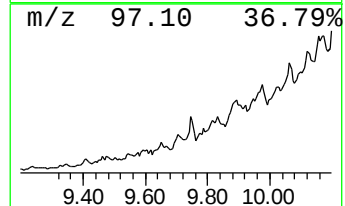
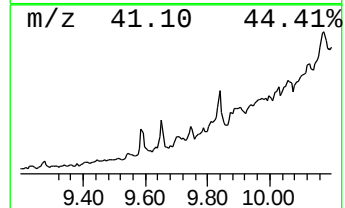
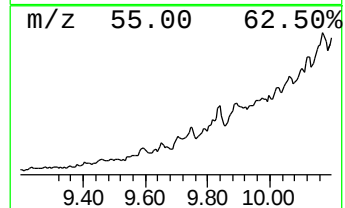
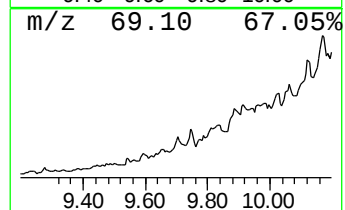
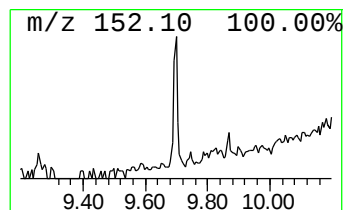
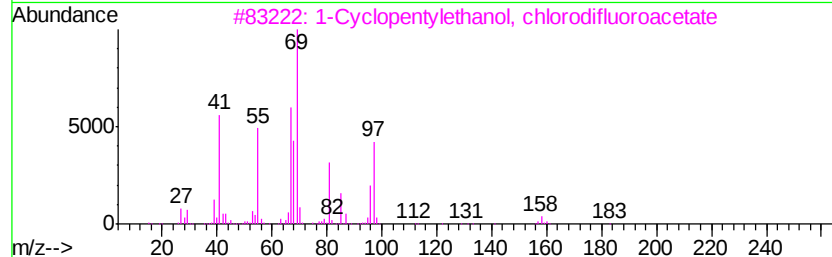
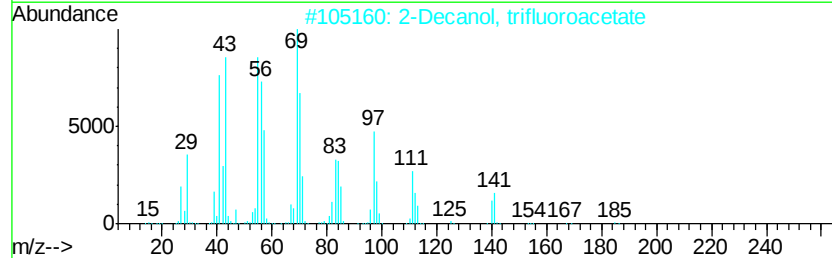
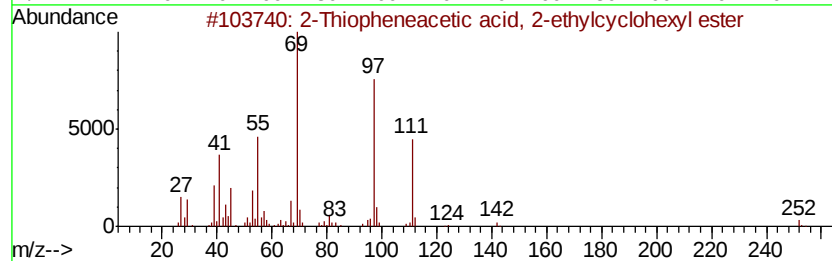
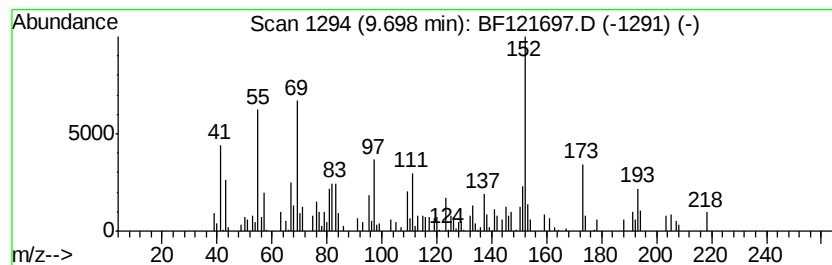
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Peak Number 4 unknown9.70 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.70	2.25 ng	128553	Acenaphthene-d10	9.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Thiopheneacetic acid, 2-ethylc...	252	C14H20O2S	1000278-96-1	38
2		2-Decanol, trifluoroacetate	254	C12H21F3O2	1000352-32-8	38
3		1-Cyclopentylethanol, chlorodifl...	226	C9H13ClF2O2	1000376-25-2	35
4		Cyclohexane, 2-ethyl-1,3-dimethyl-	140	C10H20	007045-67-2	22
5		Cyclooctane, butyl-	168	C12H24	016538-93-5	22



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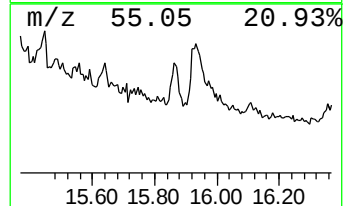
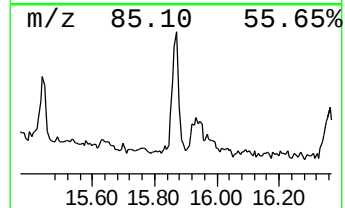
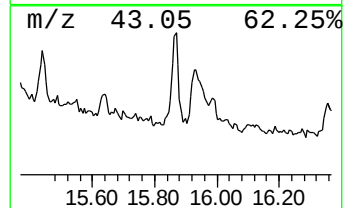
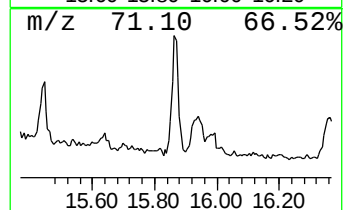
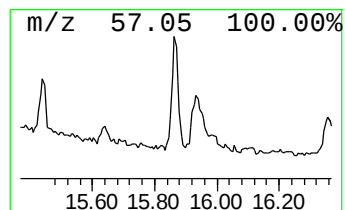
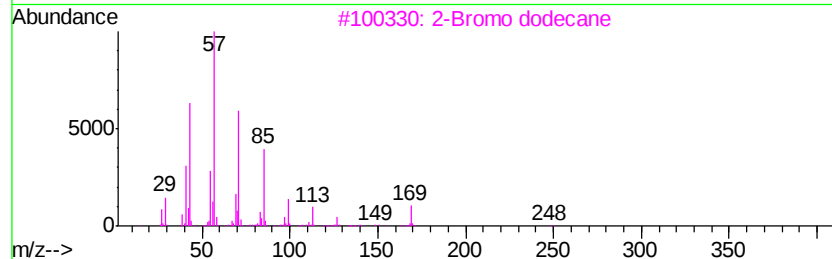
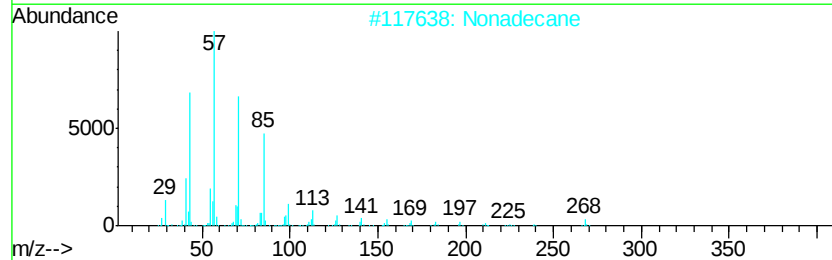
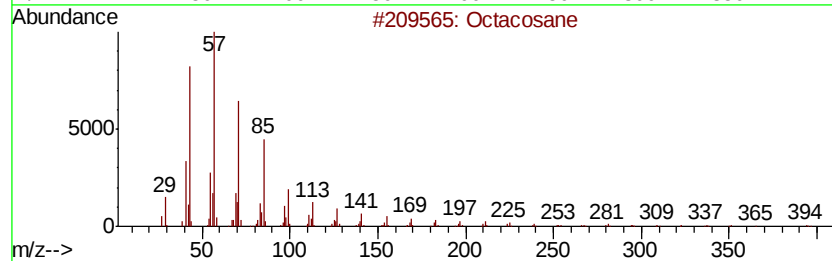
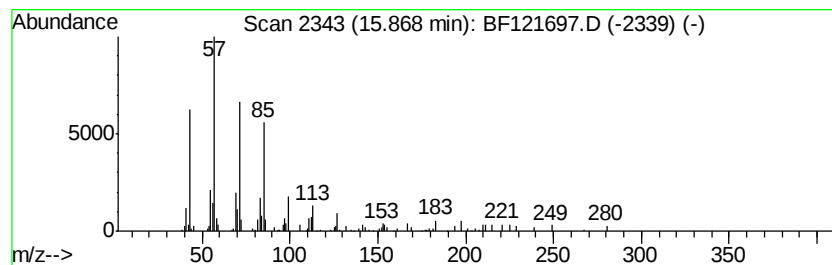
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	3.87 ng	93292	Perylene-d12	15.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	86
2	Nonadecane		268	C19H40	000629-92-5	86
3	2-Bromo dodecane		248	C12H25Br	013187-99-0	86
4	Heptadecane		240	C17H36	000629-78-7	86
5	Octadecane		254	C18H38	000593-45-3	86



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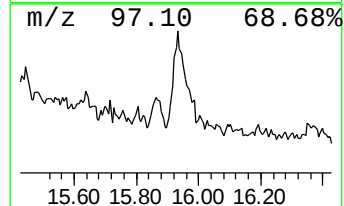
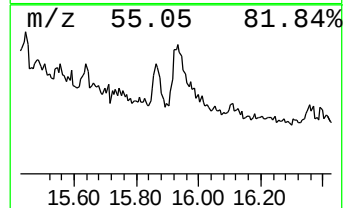
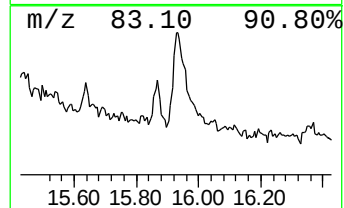
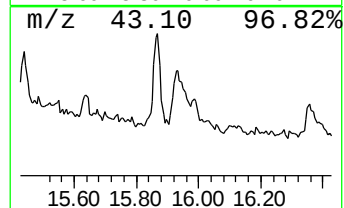
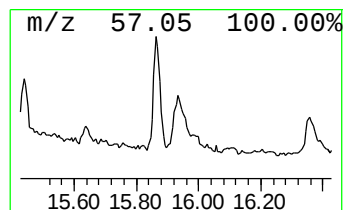
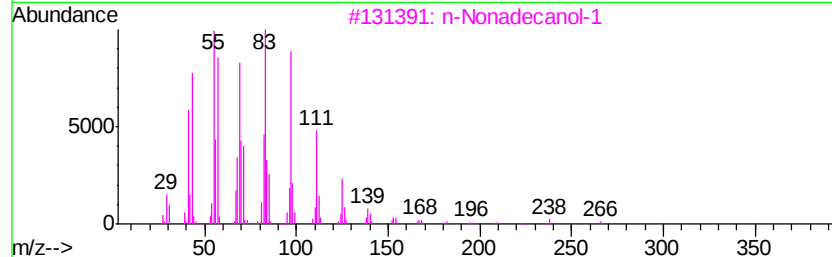
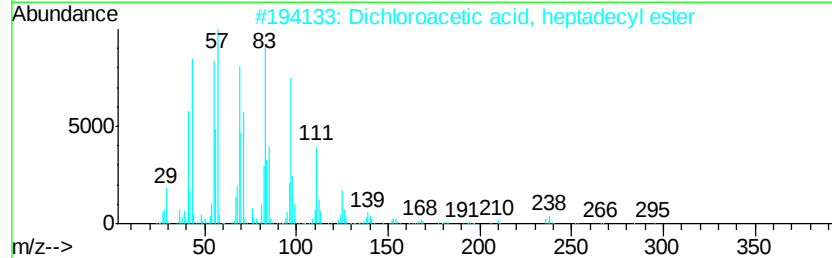
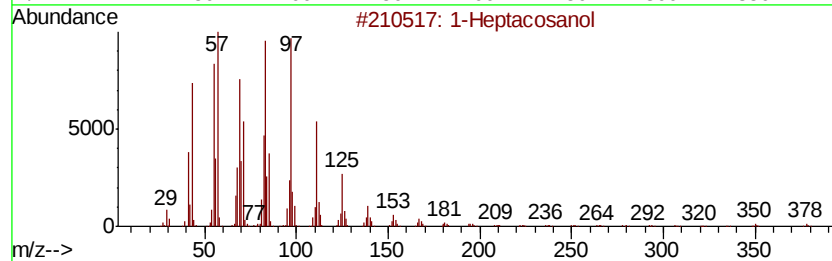
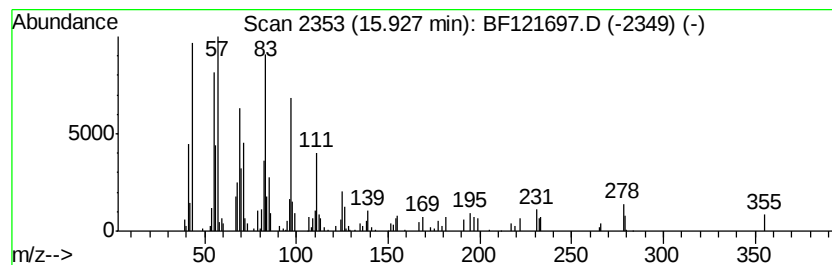
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ClientSampleId :
PE-2B-(3.0-3.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	5.59 ng	134802	Perylene-d12	15.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heptacosanol		396 C27H56O	002004-39-9 87
2	Dichloroacetic acid, heptadecyl ...		366 C19H36Cl2O2	1000282-98-2 83
3	n-Nonadecanol-1		284 C19H40O	001454-84-8 76
4	1-Heneicosanol		312 C21H44O	015594-90-8 76
5	1-Octadecanol		270 C18H38O	000112-92-5 76



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092520\
Data File : BF121697.D
Acq On : 25 Sep 2020 15:53
Operator : JU/CG
Sample : L4102-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

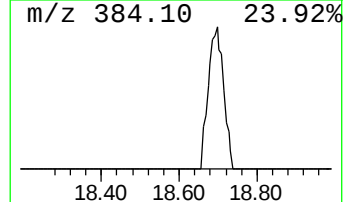
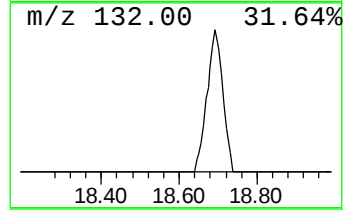
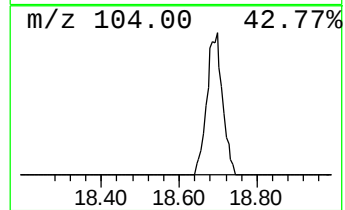
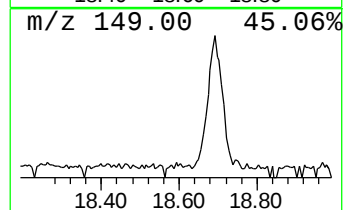
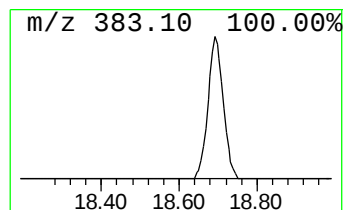
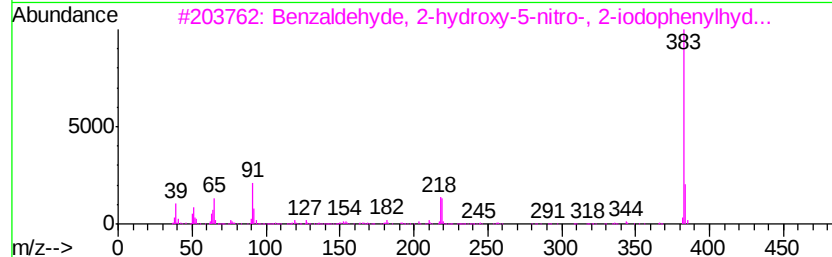
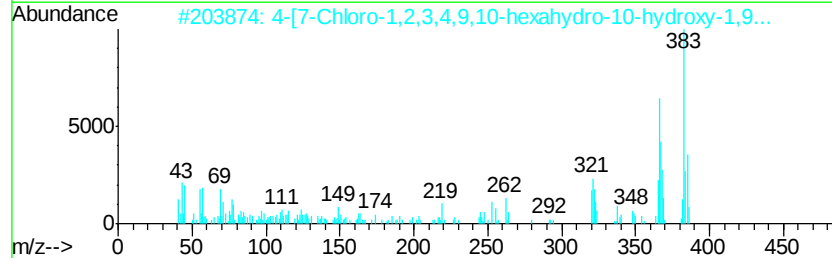
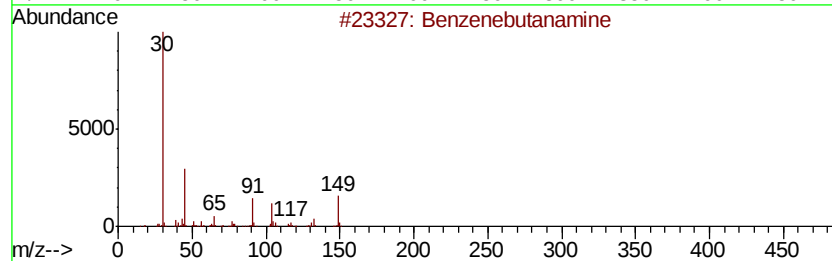
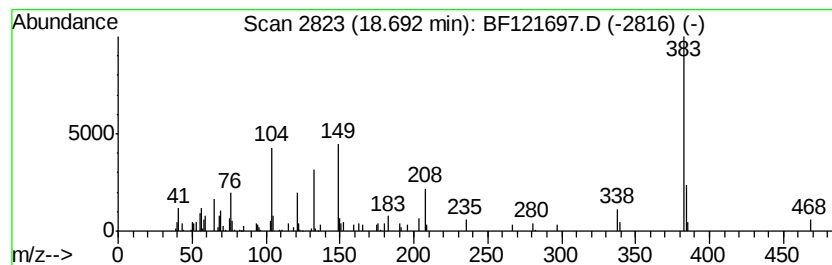
Instrument :
BNA_F
ClientSampleId :
PE-2B-(3.0-3.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown18.69 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.69	6.82 ng	164486	Perylene-d12	15.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenebutanamine	149	C10H15N	013214-66-9	22
2	4-[7-Chloro-1,2,3,4,9,10-hexahyd...	383	C20H14ClN05	075618-38-1	16
3	Benzaldehyde, 2-hydroxy-5-nitro-...	383	C13H10IN303	1000272-27-9	16
4	Purine-2,6-dione, 1,3-dimethyl-8...	383	C19H21N5O4	1000311-12-3	12
5	Iron, cyclopentadienyl-ethyl-1,2...	412	C21H42FeP2	1000156-34-1	12



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092520\
Data File : BF121697.D
Acq On : 25 Sep 2020 15:53
Operator : JU/CG
Sample : L4102-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PE-2B-(3.0-3.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	2.16	3.7	ng	87913	1	6.80	480203	20.0
2-Pentanone, 4-hy...	5.01	4.9	ng	117252	1	6.80	480203	20.0
Ethanol, 2-(2-eth...	6.63	9.4	ng	226088	1	6.80	480203	20.0
unknown9.70	9.70	2.3	ng	128553	3	9.83	1144860	20.0
Octacosane	15.87	3.9	ng	93292	6	15.42	482204	20.0
1-Heptacosanol	15.93	5.6	ng	134802	6	15.42	482204	20.0
unknown18.69	18.69	6.8	ng	164486	6	15.42	482204	20.0