

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
 Data File : BF123971.D
 Acq On : 17 May 2021 19:21
 Operator : JU/CG
 Sample : M2420-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CONCESSION-CP-3

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-BF051421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123971.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.151	5	11	16	rVB	369661	454934	39.34%	5.078%
2	2.263	26	30	34	rVB2	29295	38295	3.31%	0.427%
3	5.116	512	515	520	rVB2	15297	18432	1.59%	0.206%
4	5.516	578	583	586	rBV	949571	916497	79.25%	10.231%
5	6.522	749	754	757	rBV	1026005	949817	82.13%	10.603%
6	6.722	785	788	792	rBV	46147	34496	2.98%	0.385%
7	6.904	815	819	822	rBV	336051	263247	22.76%	2.939%
8	7.463	909	914	917	rBV	752781	621072	53.70%	6.933%
9	8.186	1033	1037	1040	rBV	419134	324639	28.07%	3.624%
10	9.263	1216	1220	1223	rBV	1508212	1128331	97.57%	12.596%
11	9.651	1283	1286	1289	rBV	137968	99481	8.60%	1.111%
12	9.939	1332	1335	1339	rVB	520360	384900	33.28%	4.297%
13	10.727	1465	1469	1472	rBV	900733	719294	62.20%	8.030%
14	11.427	1584	1588	1591	rBV	469397	378133	32.70%	4.221%
15	11.880	1659	1665	1668	rBV5	10561	14839	1.28%	0.166%
16	11.951	1674	1677	1681	rBV	108644	93649	8.10%	1.045%
17	12.639	1791	1794	1797	rBV	21851	17534	1.52%	0.196%
18	12.739	1807	1811	1814	rBV3	17124	17183	1.49%	0.192%
19	13.015	1853	1858	1861	rBV	1371368	1156471	100.00%	12.910%
20	13.909	2006	2010	2017	rBV	215586	226028	19.54%	2.523%
21	14.068	2031	2037	2040	rBV2	440371	436144	37.71%	4.869%
22	14.239	2061	2066	2070	rBV4	17441	20385	1.76%	0.228%
23	14.545	2115	2118	2122	rBV3	36280	46985	4.06%	0.524%
24	14.704	2141	2145	2150	rVB3	30680	34344	2.97%	0.383%
25	14.939	2182	2185	2189	rBV4	31099	32759	2.83%	0.366%
26	15.115	2213	2215	2219	rBV3	15689	26198	2.27%	0.292%
27	15.204	2226	2230	2233	rBV5	20789	27335	2.36%	0.305%
28	15.562	2285	2291	2295	rBV	303215	354391	30.64%	3.956%
29	15.598	2295	2297	2301	rVB4	19466	21400	1.85%	0.239%
30	16.056	2371	2375	2378	rVB5	14453	15523	1.34%	0.173%
31	16.103	2379	2383	2389	rVB7	28822	52354	4.53%	0.584%
32	16.303	2413	2417	2422	rVB7	12462	18441	1.59%	0.206%
33	16.621	2467	2471	2474	rVB4	10616	14602	1.26%	0.163%

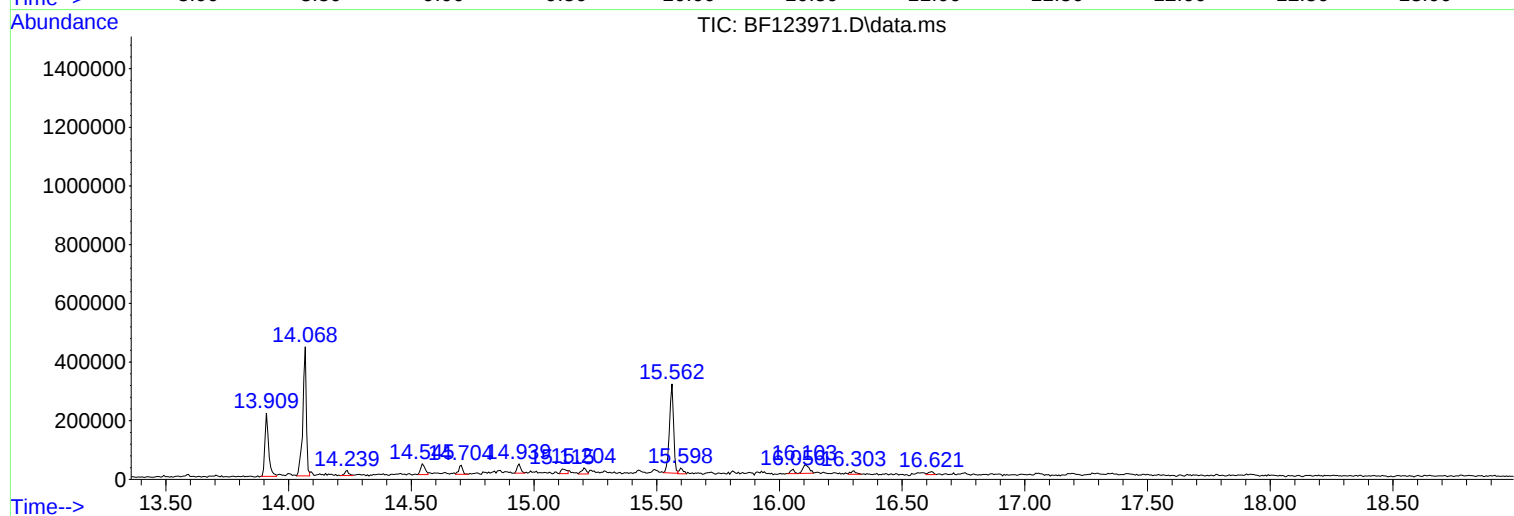
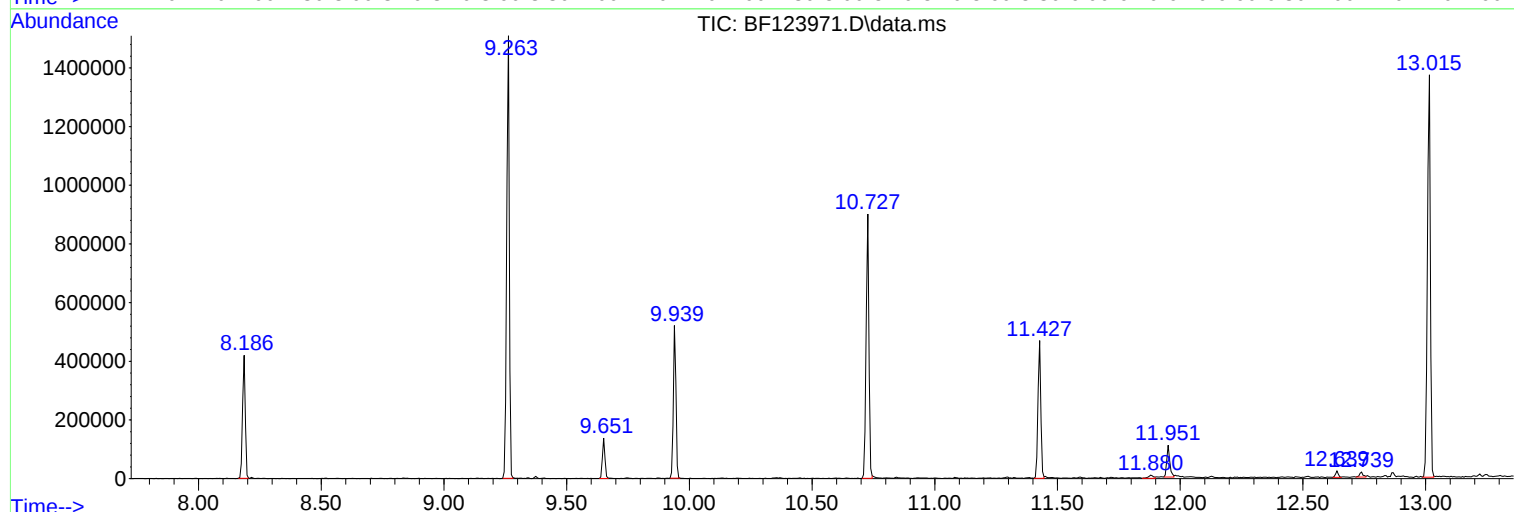
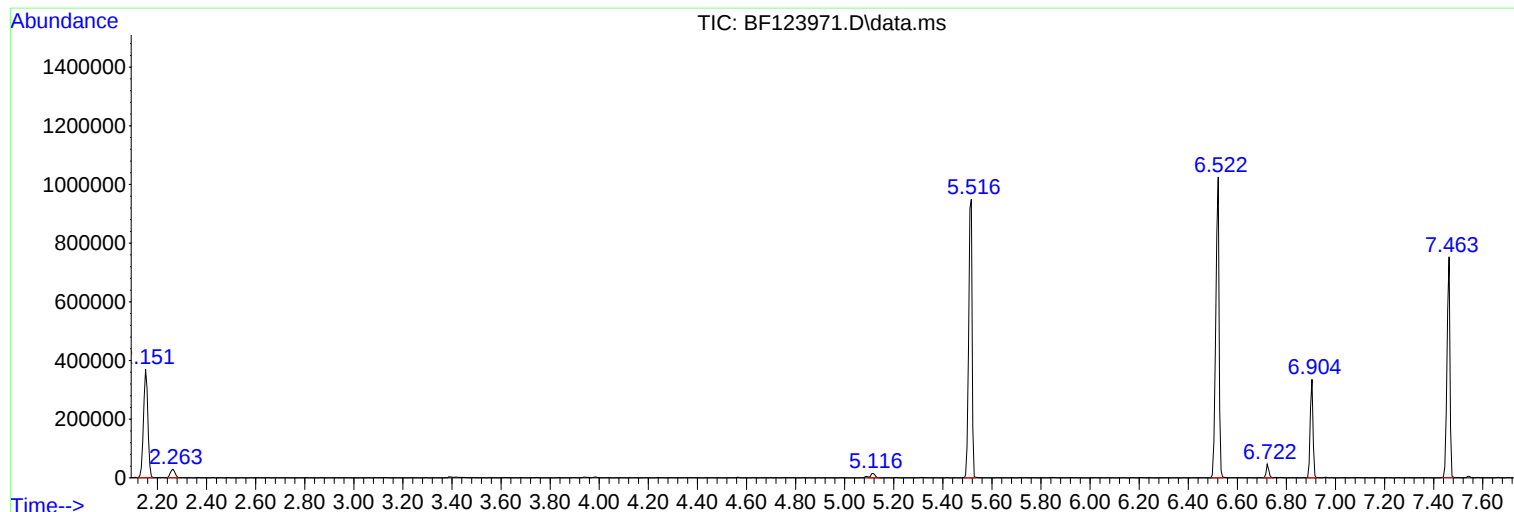
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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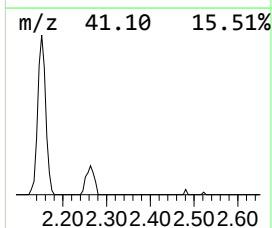
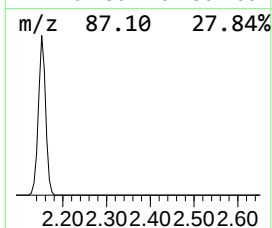
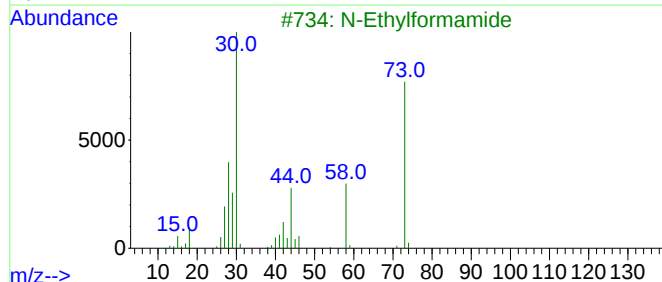
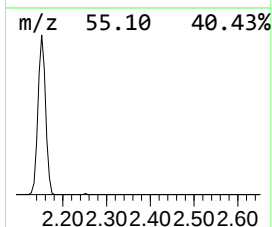
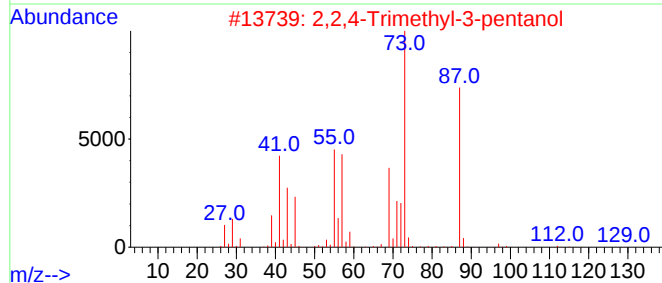
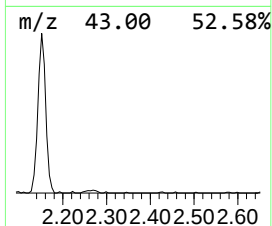
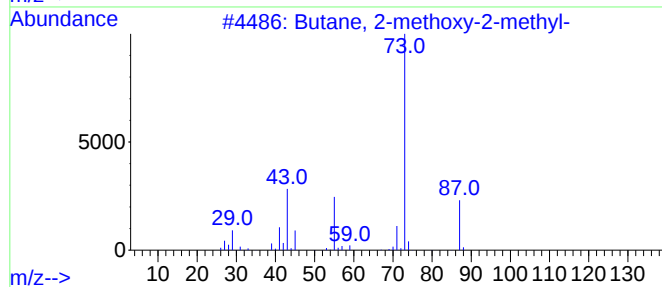
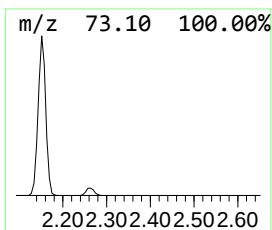
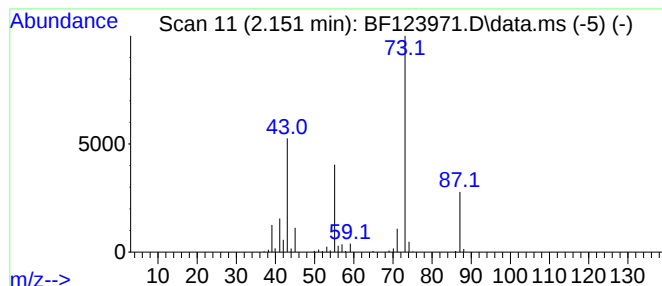
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.151	34.56 ng	454934	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			N-Ethylformamide	73	C3H7NO	000627-45-2	9
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			1-Butanol, 2-methyl-, acetate	130	C7H14O2	000624-41-9	9



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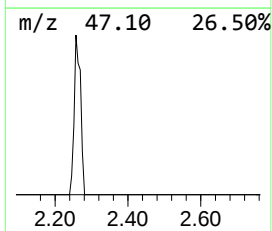
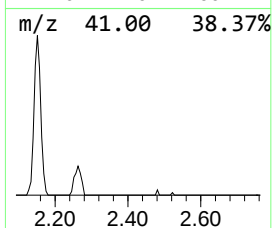
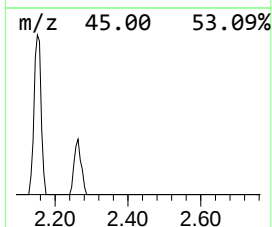
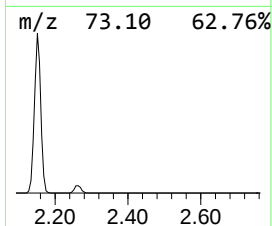
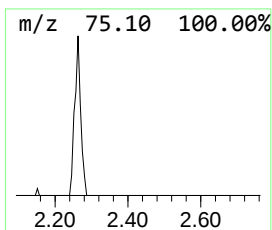
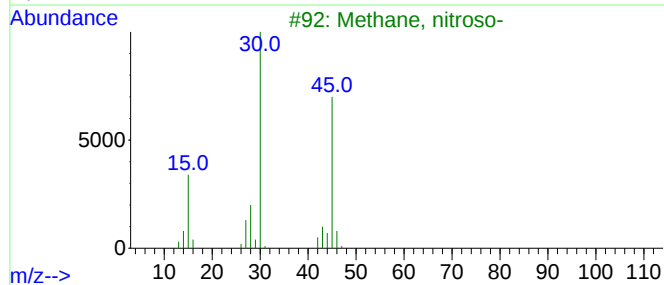
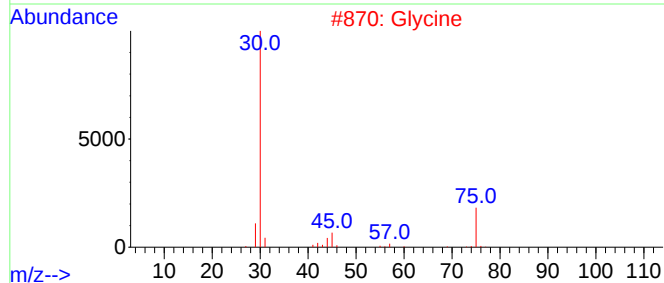
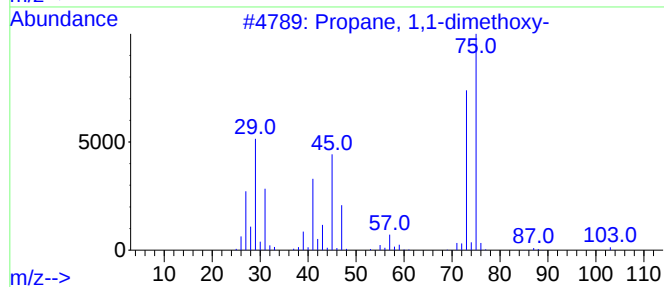
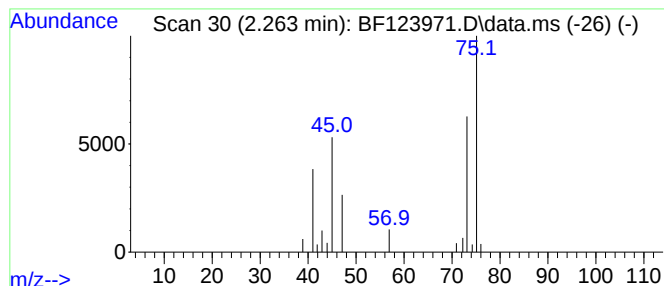
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.263	2.91 ng	38295	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2			Glycine	75	C2H5NO2	000056-40-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	5
4			Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	4
5			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	4



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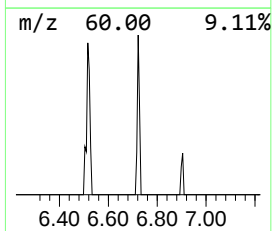
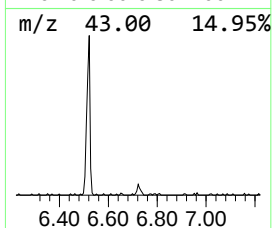
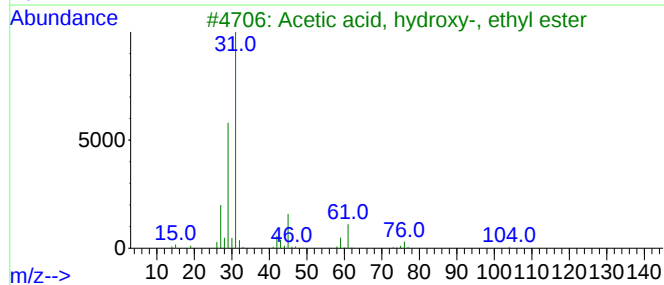
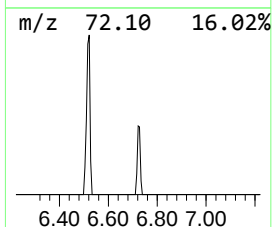
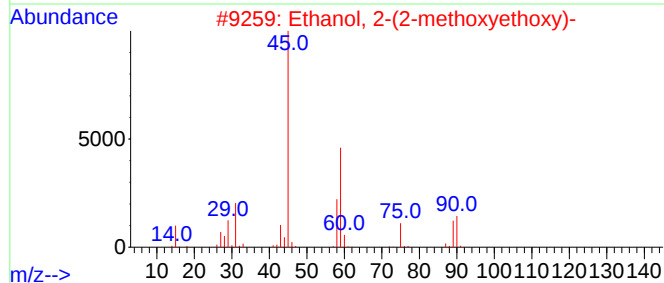
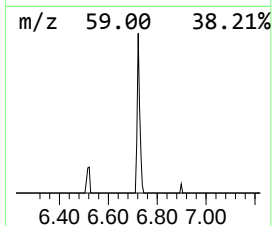
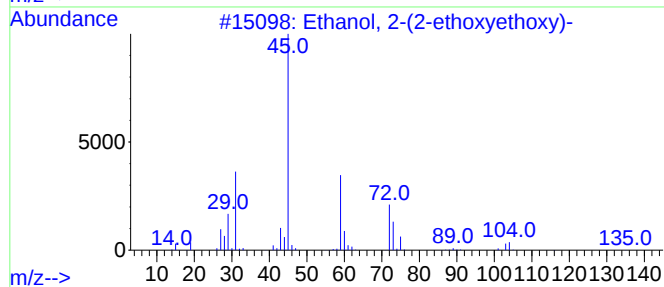
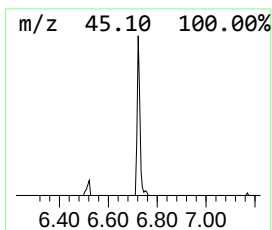
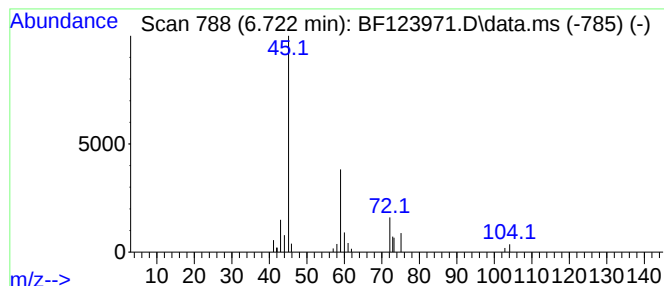
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.722	2.62 ng	34496	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	50
3			Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	45
4			2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	39
5			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38



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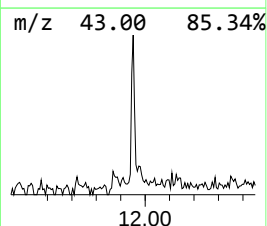
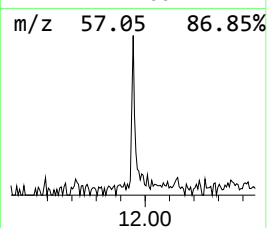
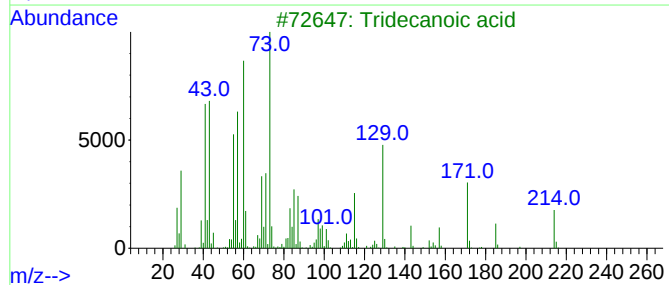
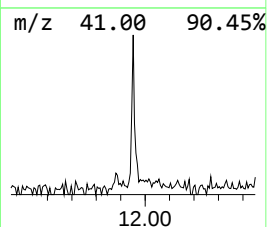
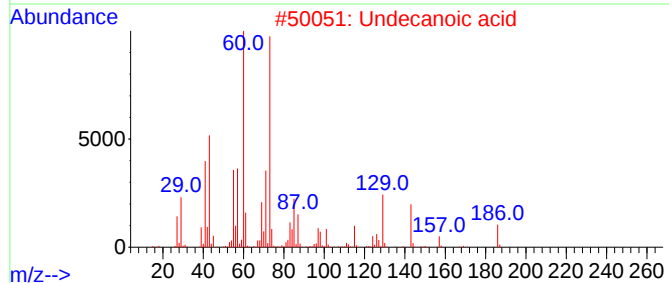
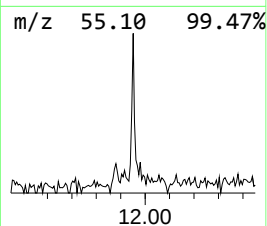
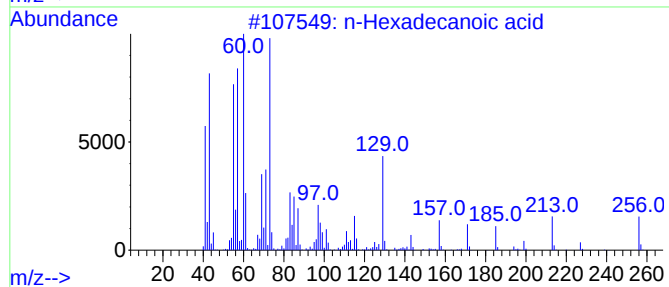
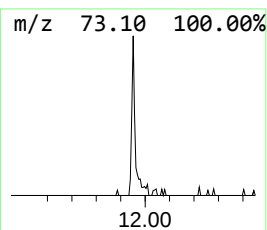
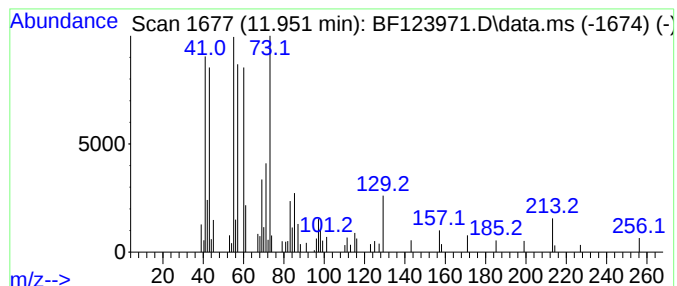
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	4.95 ng	93649	Phenanthrene-d10	11.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Undecanoic acid	186	C11H22O2	000112-37-8	86
3			Tridecanoic acid	214	C13H26O2	000638-53-9	86
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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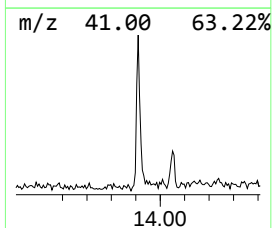
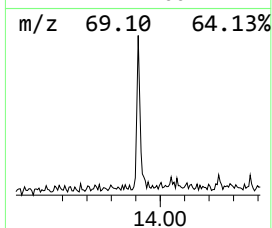
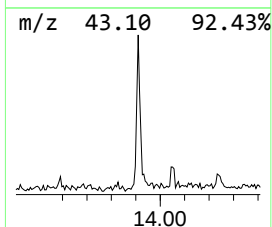
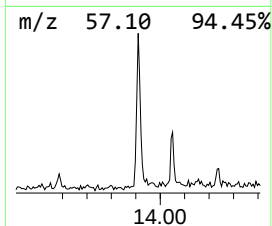
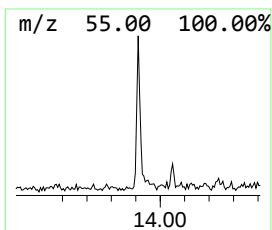
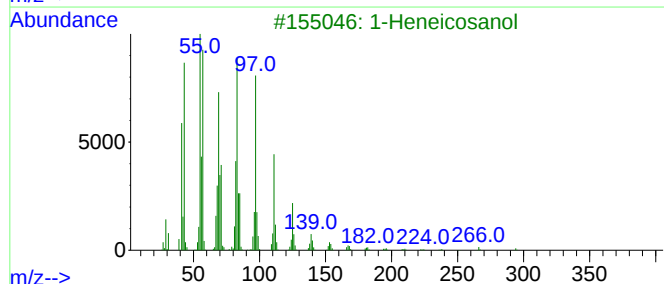
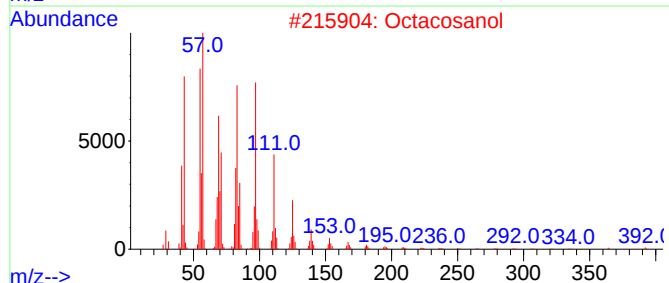
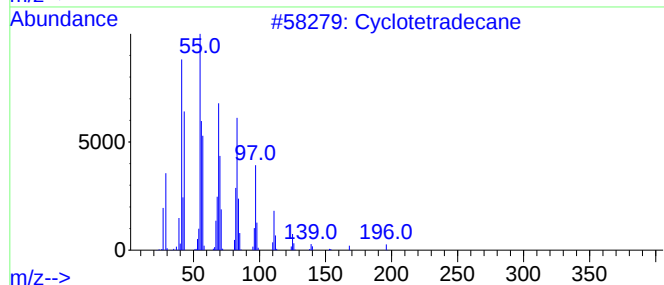
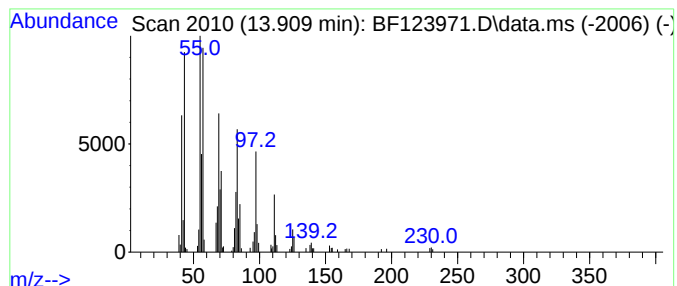
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Peak Number 5 Cyclotetradecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	10.36 ng	226028	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	93
2			Octacosanol	410	C28H58O	000557-61-9	91
3			1-Heneicosanol	312	C21H44O	015594-90-8	91
4			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



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ClientSampleId :
CONCESSION-CP-3

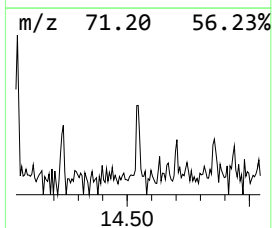
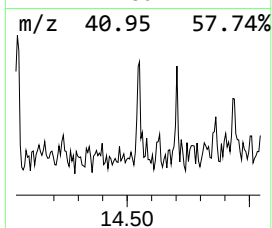
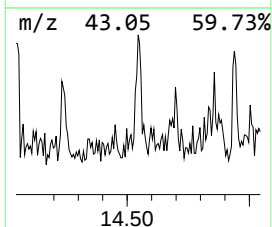
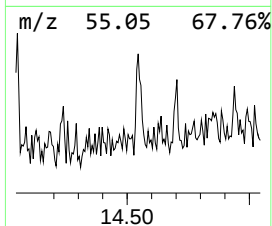
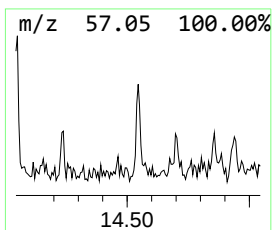
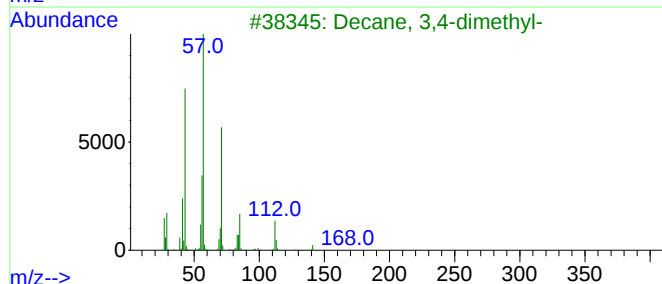
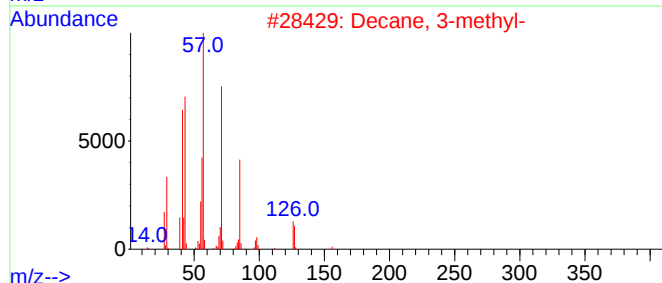
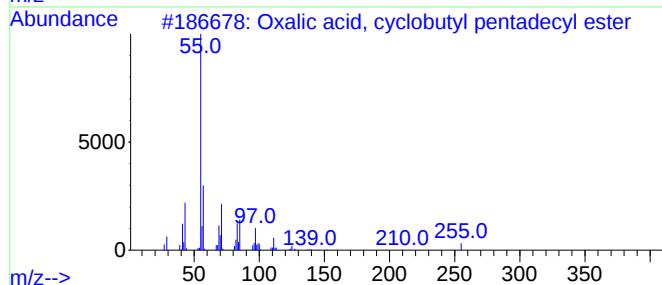
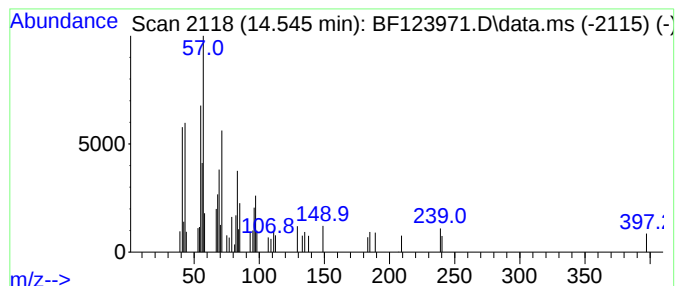
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.545 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.545	2.15 ng	46985	Chrysene-d12	14.068

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	43
2			Decane, 3-methyl-	156	C11H24	013151-34-3	43
3			Decane, 3,4-dimethyl-	170	C12H26	017312-45-7	43
4			Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	35
5			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123971.D
Acq On : 17 May 2021 19:21
Operator : JU/CG
Sample : M2420-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

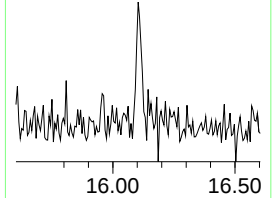
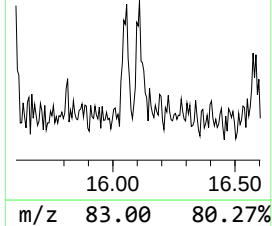
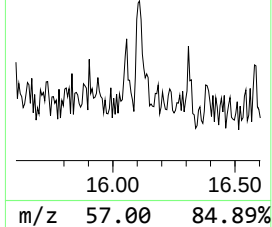
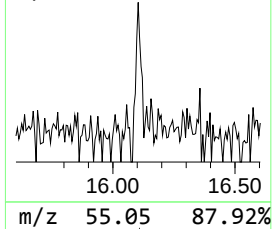
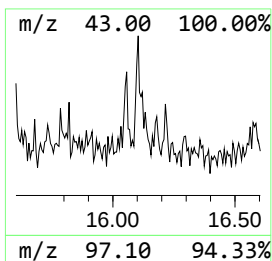
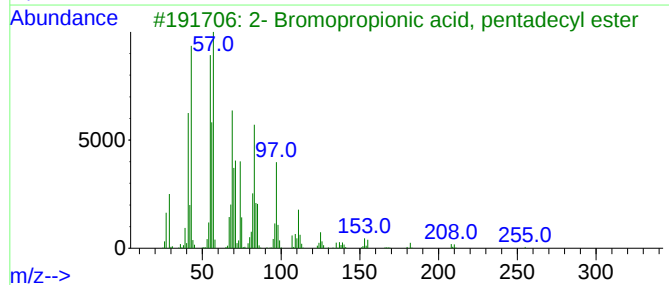
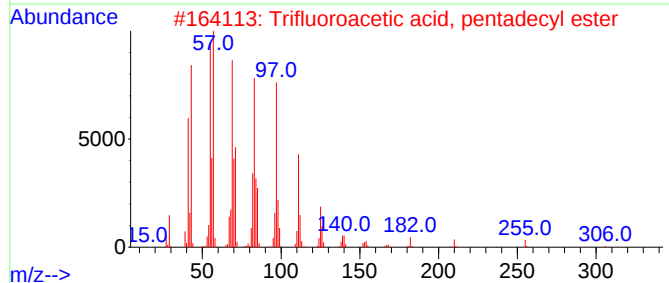
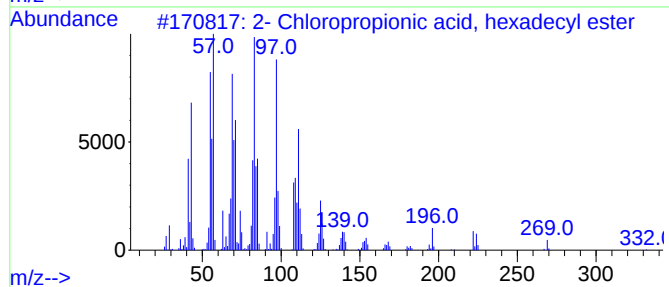
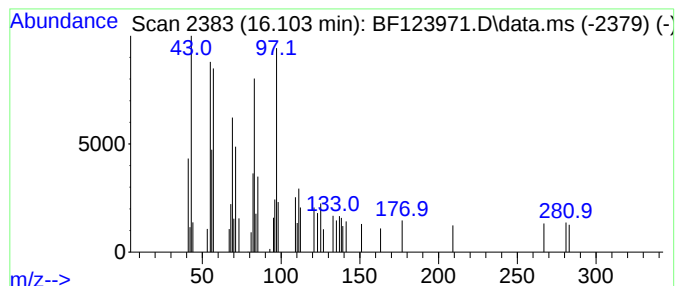
Instrument :
BNA_F
ClientSampleId :
CONCESSION-CP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2- Chloropropionic acid, he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.104	2.95 ng	52354	Perylene-d12	15.562	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	78
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	72
3	2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	72
4	Octacosyl acetate	452	C30H60O2	018206-97-8	68
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123971.D
Acq On : 17 May 2021 19:21
Operator : JU/CG
Sample : M2420-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCESSION-CP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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
Butane, 2-metho...	2.151	34.6	ng	454934	1	6.904	263247	20.0
Propane, 1,1-di...	2.263	2.9	ng	38295	1	6.904	263247	20.0
Ethanol, 2-(2-e...	6.722	2.6	ng	34496	1	6.904	263247	20.0
n-Hexadecanoic ...	11.951	5.0	ng	93649	4	11.427	378133	20.0
Cyclotetradecane	13.910	10.4	ng	226028	5	14.068	436144	20.0
unknown14.545	14.545	2.1	ng	46985	5	14.068	436144	20.0
2- Chloropropio...	16.104	3.0	ng	52354	6	15.562	354391	20.0