

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031524\
 Data File : BF137615.D
 Acq On : 15 Mar 2024 18:08
 Operator : CG\JU
 Sample : P1747-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-01

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137615.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.899	474	478	489	rBV	297420	343093	7.72%	1.490%
2	5.328	547	551	568	rBV	1072182	1147604	25.82%	4.984%
3	6.357	723	726	742	rBV	645729	714142	16.07%	3.101%
4	6.722	785	788	797	rBV	848221	739958	16.65%	3.213%
5	6.787	797	799	805	rVB	64169	71812	1.62%	0.312%
6	7.292	880	885	896	rBV	2658110	2470694	55.59%	10.729%
7	8.004	1003	1006	1016	rBV	1150516	994091	22.37%	4.317%
8	8.539	1094	1097	1106	rVB	113789	109315	2.46%	0.475%
9	9.086	1185	1190	1193	rBV	4637629	4359381	98.08%	18.931%
10	9.757	1300	1304	1316	rVV	1456936	1172306	26.38%	5.091%
11	9.857	1316	1321	1327	rVB	95936	96557	2.17%	0.419%
12	10.139	1365	1369	1372	rBV	180438	143364	3.23%	0.623%
13	10.392	1408	1412	1423	rBV	353471	369579	8.32%	1.605%
14	10.545	1434	1438	1449	rBV	2103170	1900975	42.77%	8.255%
15	11.239	1552	1556	1563	rBV	1412403	1210570	27.24%	5.257%
16	11.328	1569	1571	1577	rBV2	48031	52524	1.18%	0.228%
17	11.775	1643	1647	1651	rBV	153335	183239	4.12%	0.796%
18	12.557	1777	1780	1787	rBV2	47775	71552	1.61%	0.311%
19	12.827	1822	1826	1829	rBV	4808844	4444566	100.00%	19.301%
20	13.733	1974	1980	1990	rBV3	86237	141438	3.18%	0.614%
21	13.874	2000	2004	2011	rBV	1192934	1077149	24.24%	4.678%
22	14.463	2100	2104	2109	rBV	197159	201560	4.53%	0.875%
23	15.298	2241	2246	2260	rBV	674700	922550	20.76%	4.006%
24	16.221	2398	2403	2419	rVB9	35309	89377	2.01%	0.388%

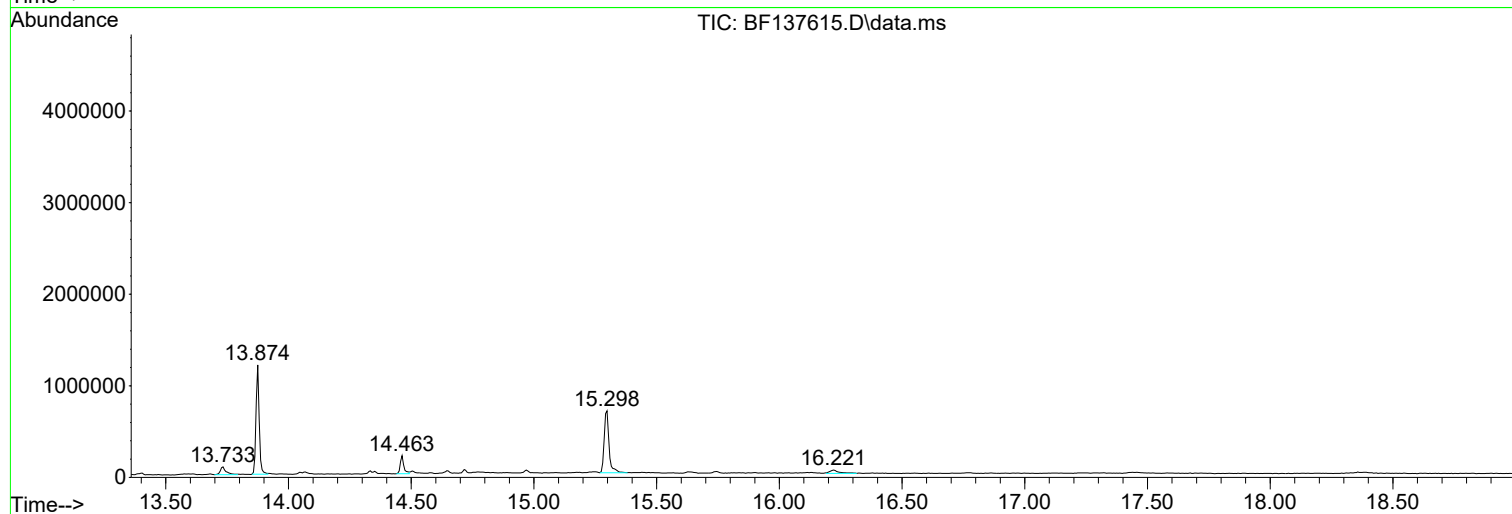
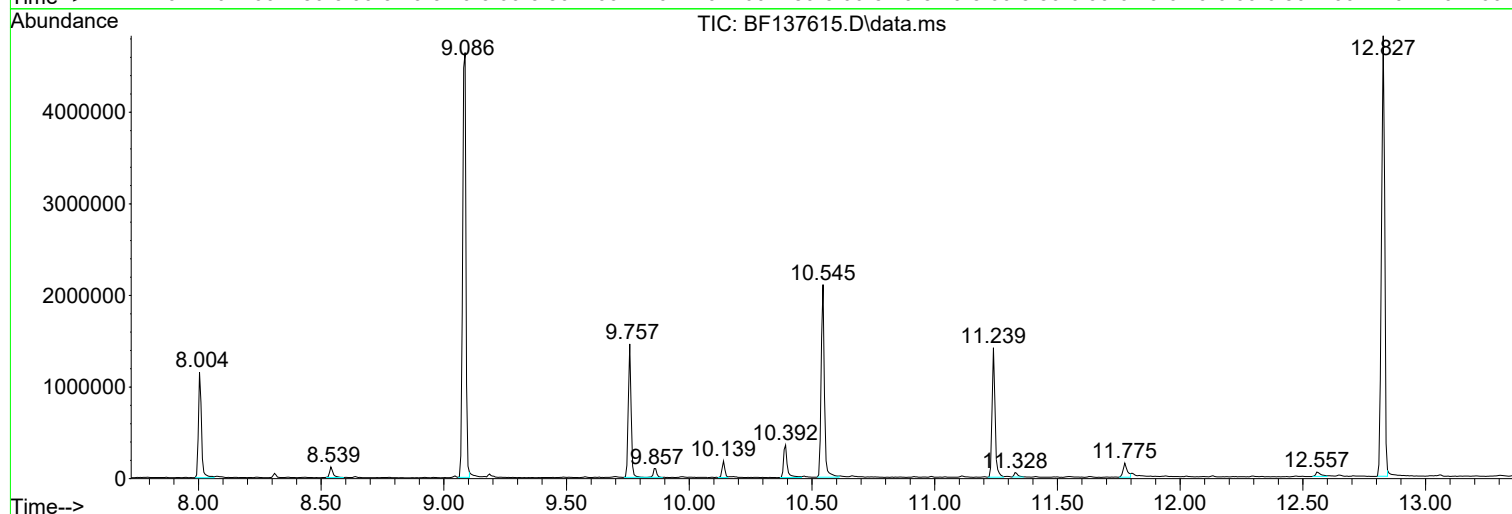
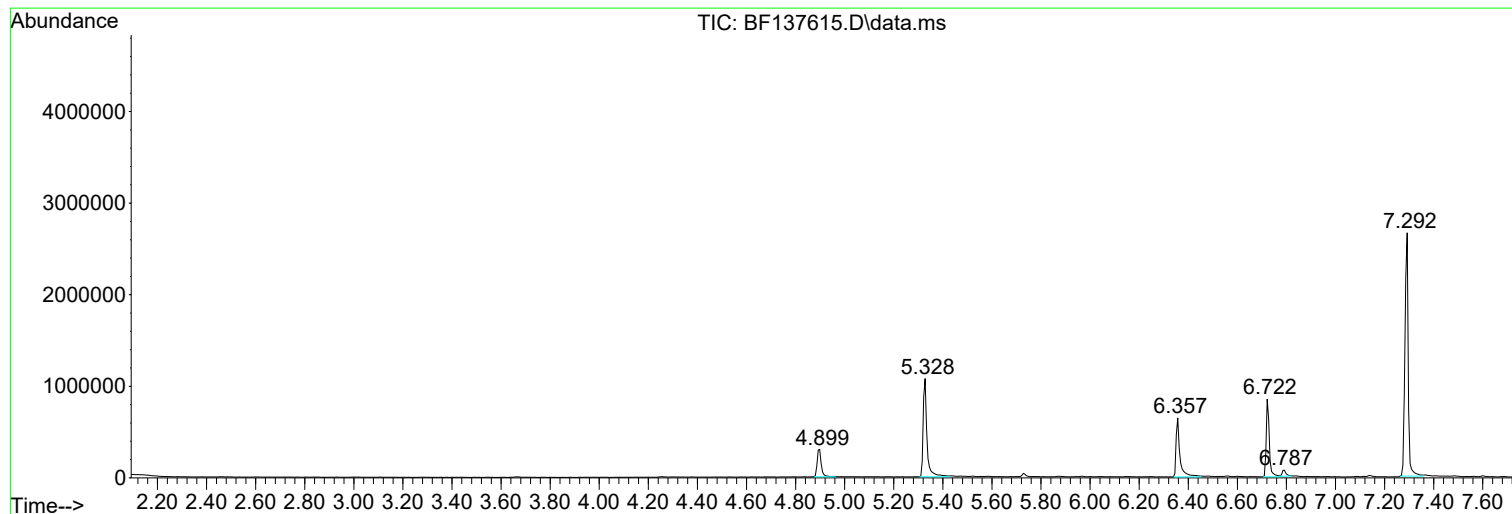
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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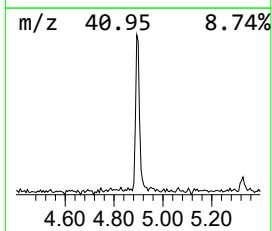
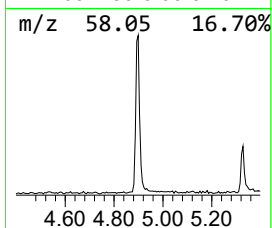
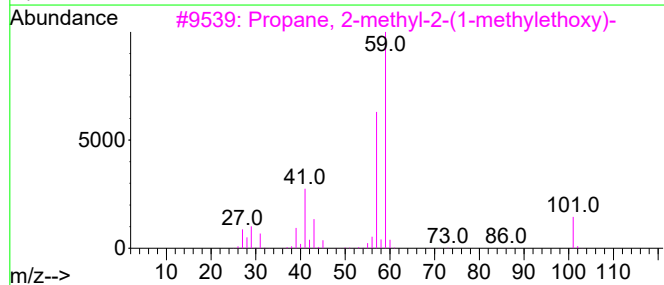
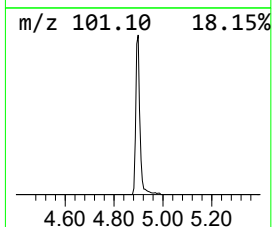
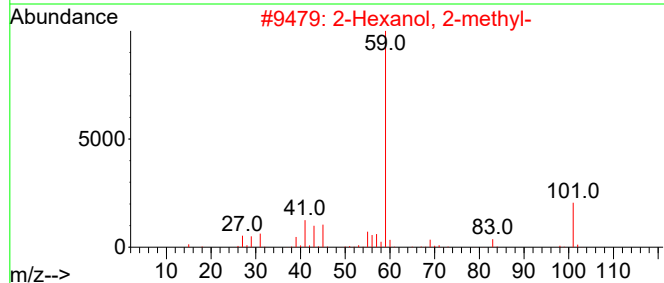
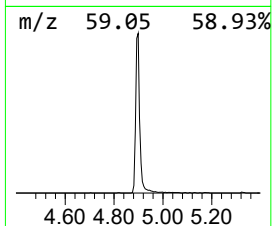
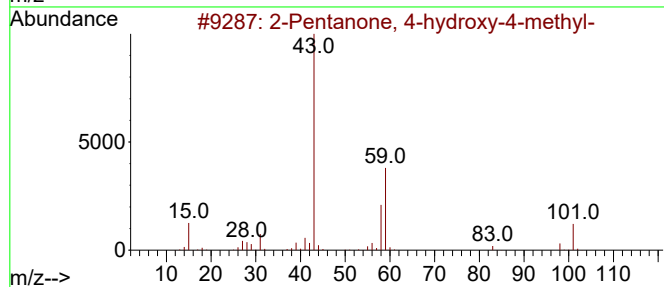
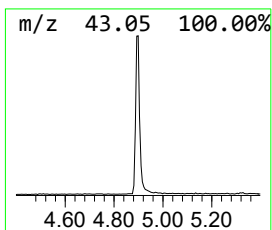
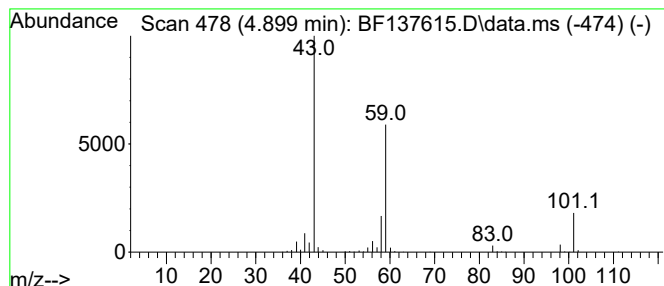
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.899	9.27 ng	343093	1,4-Dichlorobenzene-d4	6.722

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	38		
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		



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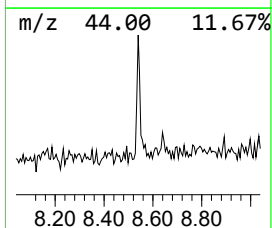
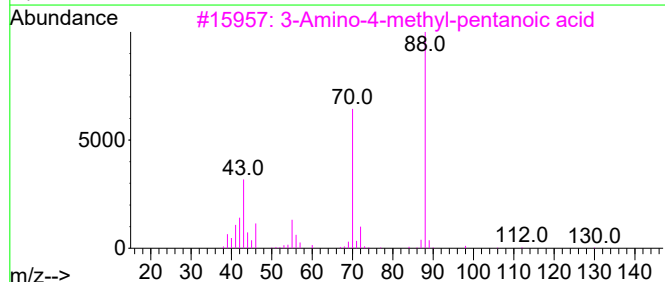
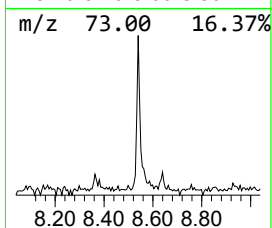
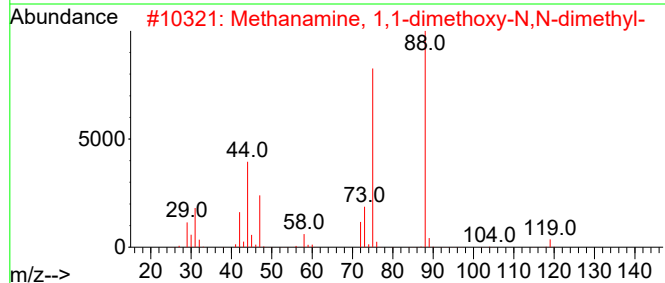
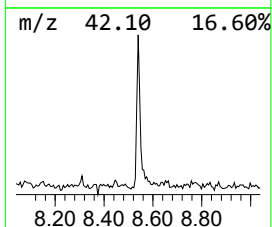
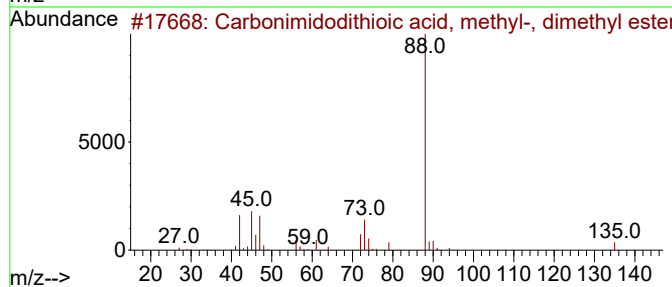
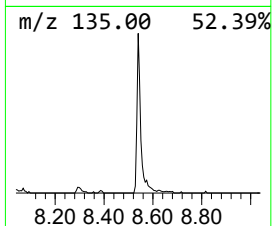
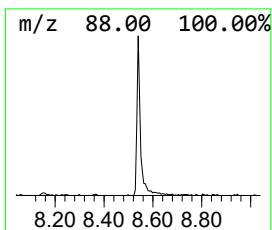
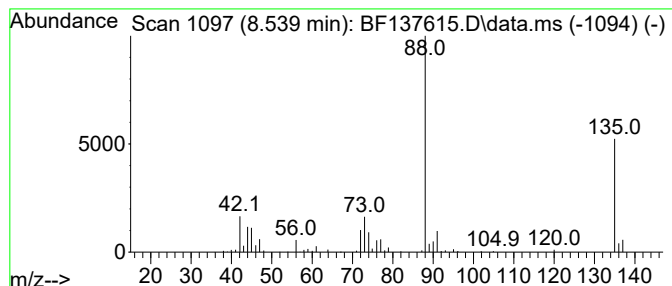
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Peak Number 2 Carbonimidodithioic acid, m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.539	2.20 ng	109315	Naphthalene-d8	8.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonimidodithioic acid, methyl...	135	C4H9NS2	018805-25-9	50
2			Methanamine, 1,1-dimethoxy-N,N-d...	119	C5H13NO2	004637-24-5	47
3			3-Amino-4-methyl-pentanoic acid	131	C6H13NO2	005699-54-7	37
4			Dithiocarbamic acid, N,N-dimethy...	164	C5H12N2S2	002801-22-1	37
5			Hydroxyethyl-3,4-methylenedioxa...	223	C12H17NO3	1000378-95-1	36



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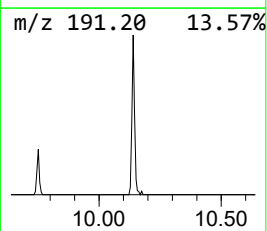
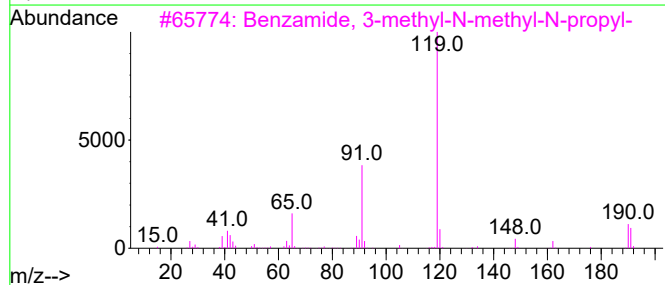
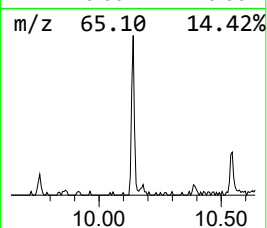
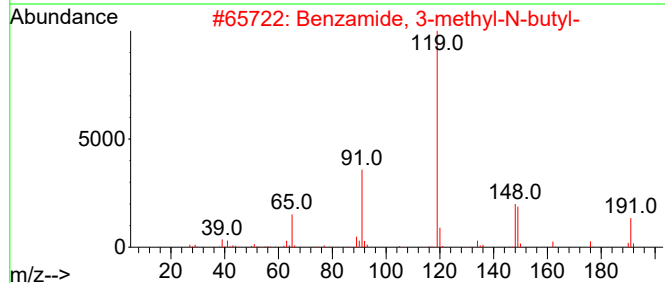
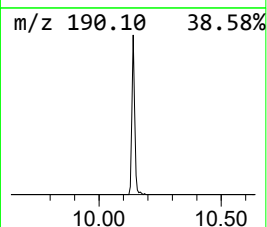
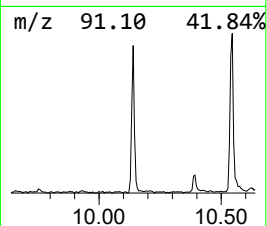
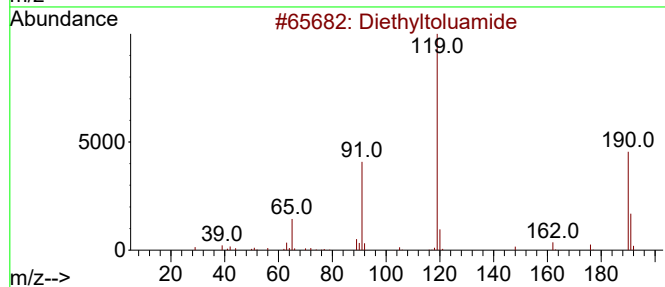
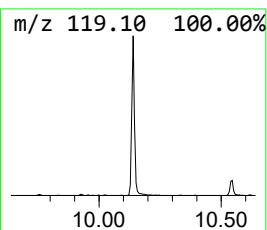
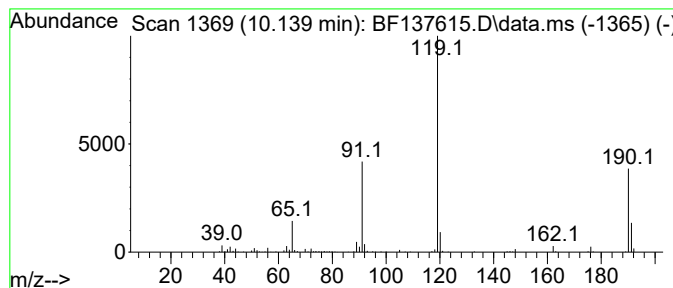
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Peak Number 3 Diethyltoluamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.139	2.45 ng	143364	Acenaphthene-d10	9.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethyltoluamide	191	C12H17NO	000134-62-3	97
2			Benzamide, 3-methyl-N-butyl-	191	C12H17NO	1000407-41-1	76
3			Benzamide, 3-methyl-N-methyl-N-p...	191	C12H17NO	1000421-46-2	72
4			Benzamide, 4-methyl-N-butyl-	191	C12H17NO	1000407-46-6	68
5			Benzamide, 3-methyl-N-isobutyl-	191	C12H17NO	1000407-41-0	68



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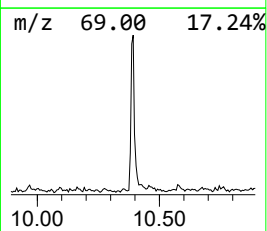
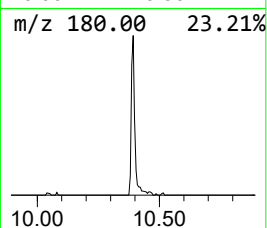
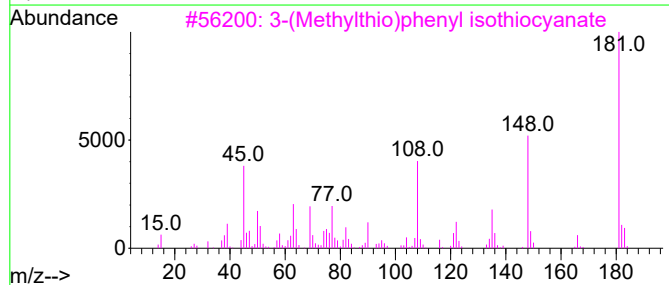
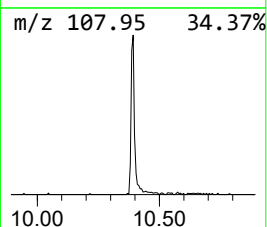
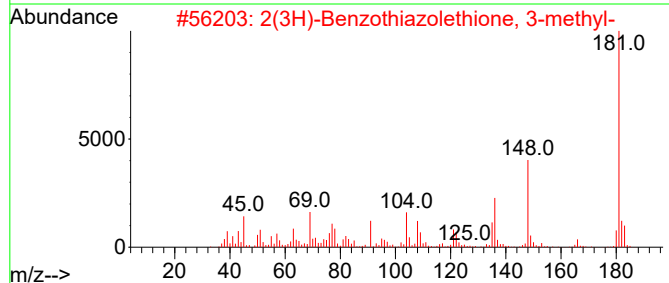
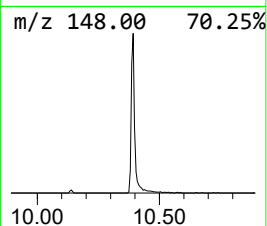
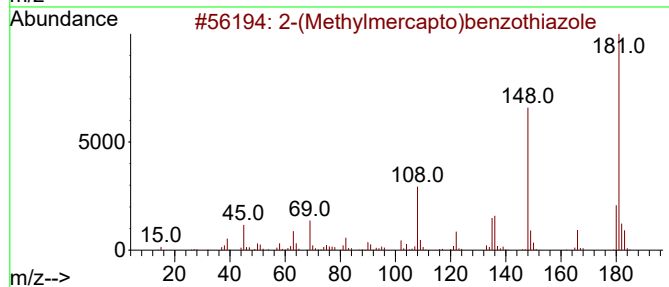
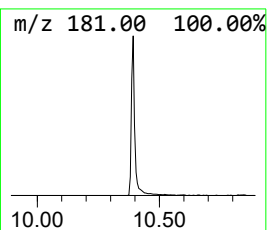
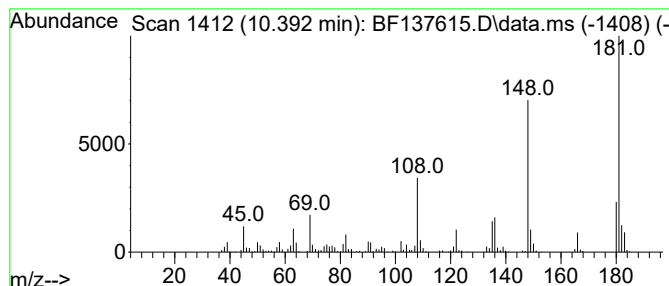
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 2-(Methylmercapto)benzothia... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.392	6.31 ng	369579	Acenaphthene-d10	9.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-(Methylmercapto)benzothiazole	181	C8H7NS2	000615-22-5	99
2			2(3H)-Benzothiazolethione, 3-met...	181	C8H7NS2	002254-94-6	87
3			3-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	051333-80-3	83
4			2-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	051333-75-6	74
5			Acetonitrile, (3-chloro-5,5-dime...	181	C10H12ClN	076399-17-2	46



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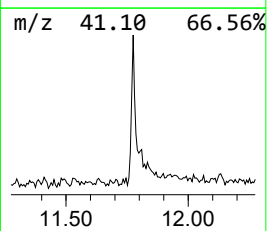
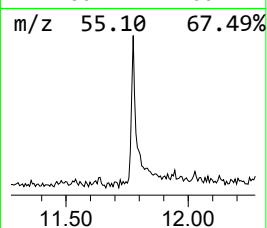
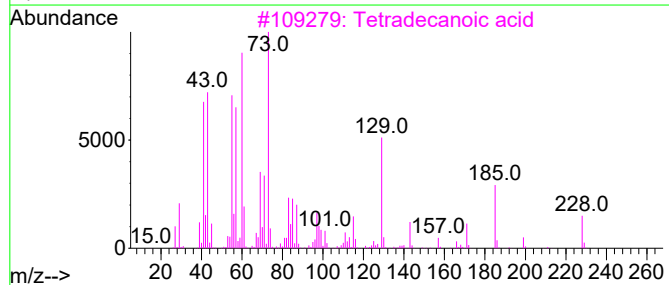
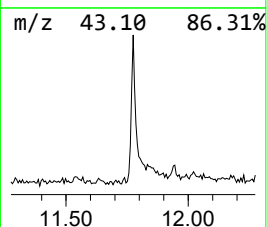
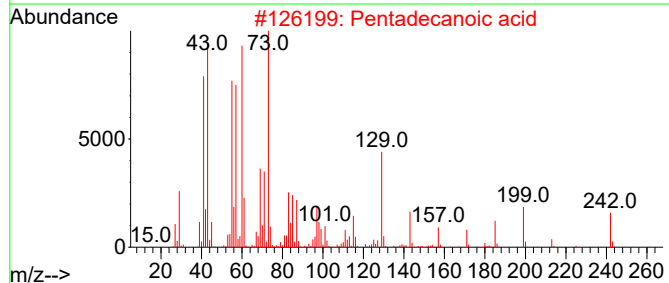
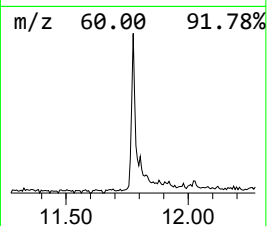
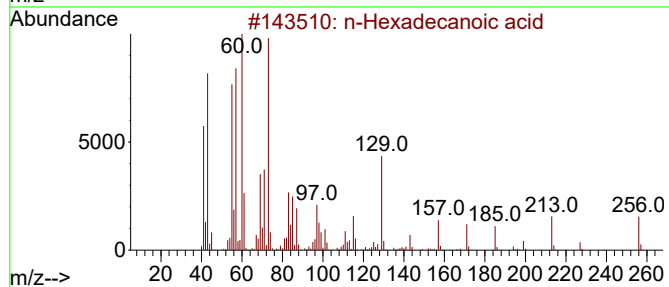
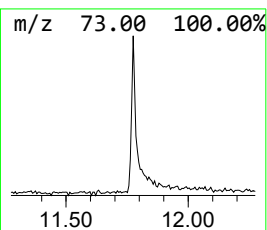
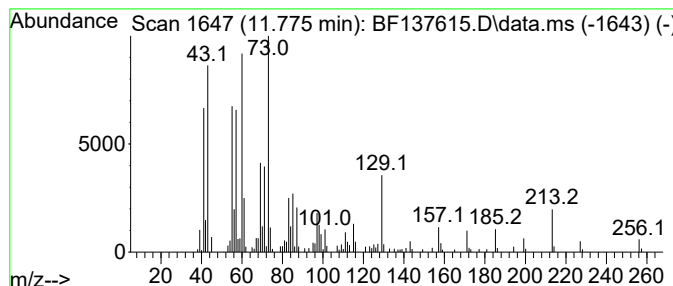
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.775	3.03 ng	183239	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	90
5			Nonanoic acid	158	C9H18O2	000112-05-0	43



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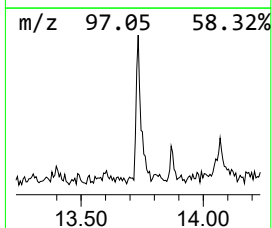
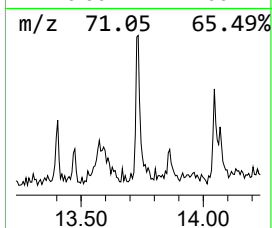
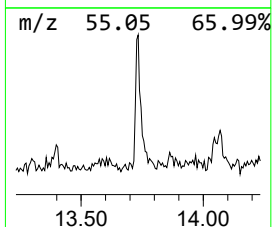
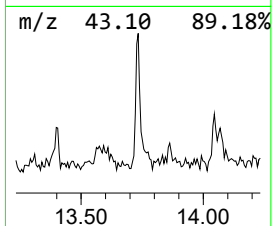
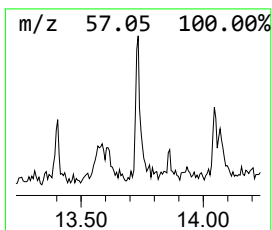
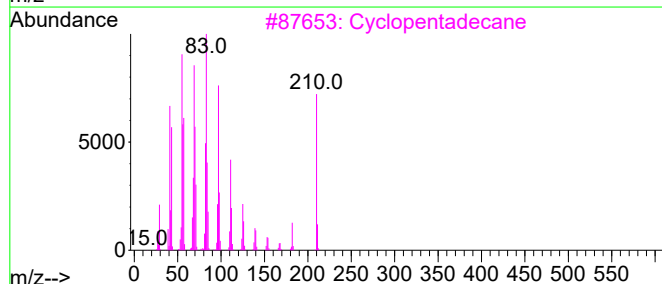
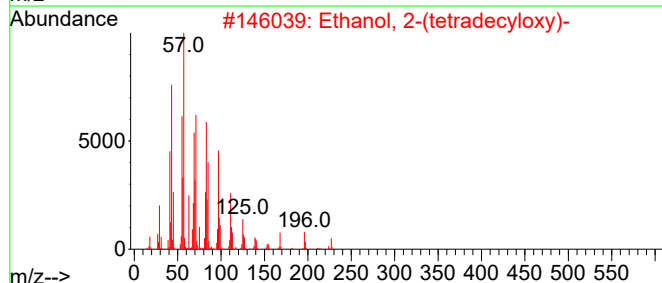
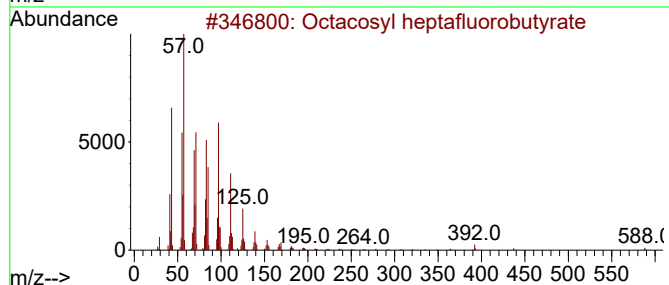
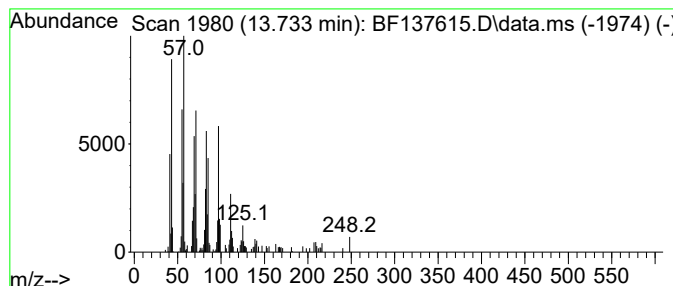
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octacosyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.733	2.63 ng	141438	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	87
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
3			Cyclopentadecane	210	C15H30	000295-48-7	81
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	76
5			1-Heptacosanol	396	C27H56O	002004-39-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031524\
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Acq On : 15 Mar 2024 18:08
Operator : CG\JU
Sample : P1747-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

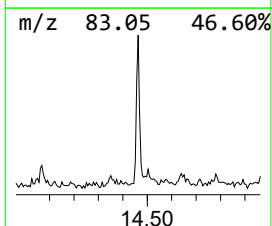
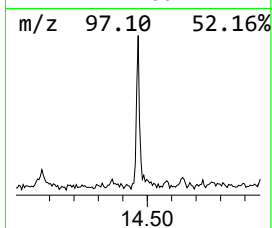
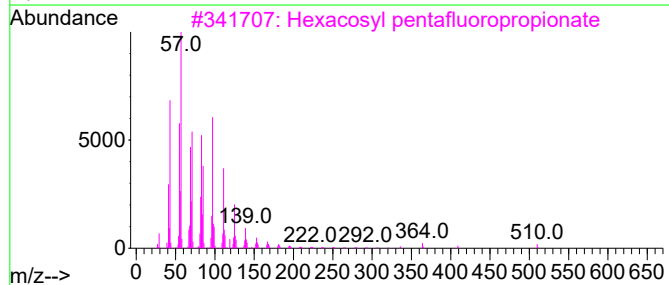
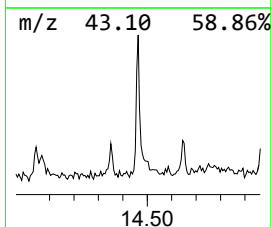
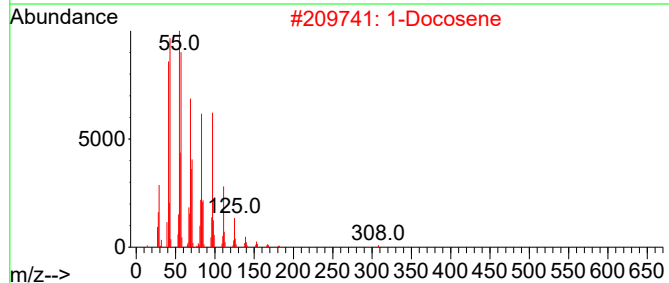
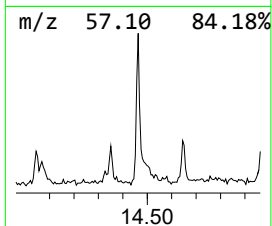
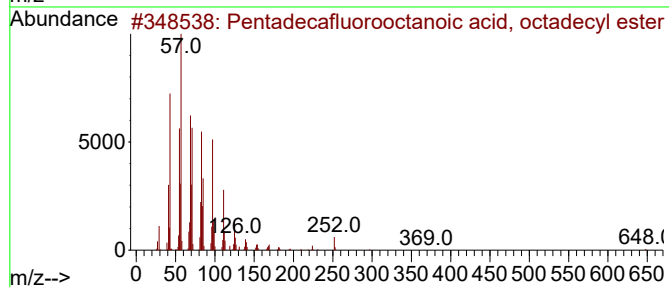
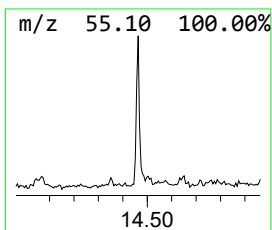
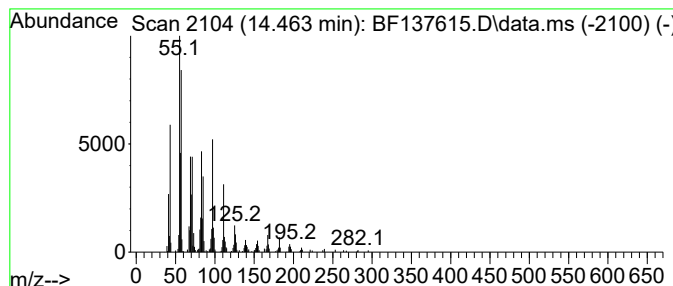
Instrument :
BNA_F
ClientSampleId :
MW-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.463	3.74 ng	201560	Chrysene-d12	13.874	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2	1-Docosene	308	C22H44	001599-67-3	91
3	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	87
4	Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	87
5	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031524\
Data File : BF137615.D
Acq On : 15 Mar 2024 18:08
Operator : CG\JU
Sample : P1747-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.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
2-Pentanone, 4-...	4.899	9.3	ng	343093	1	6.722	739958	20.0
Carbonimidodith...	8.539	2.2	ng	109315	2	8.004	994091	20.0
Diethyltoluamide	10.139	2.5	ng	143364	3	9.757	1172310	20.0
2-(Methylmercap...	10.392	6.3	ng	369579	3	9.757	1172310	20.0
n-Hexadecanoic ...	11.775	3.0	ng	183239	4	11.239	1210570	20.0
Octacosyl hepta...	13.733	2.6	ng	141438	5	13.874	1077150	20.0
Pentadecafluoro...	14.463	3.7	ng	201560	5	13.874	1077150	20.0