

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020323\
 Data File : BF132325.D
 Acq On : 03 Feb 2023 16:59
 Operator : CG\JU
 Sample : 01371-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 4-RAMP-E

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-BF013123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132325.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.313	414	421	432	rVB	1337854	1854731	33.48%	4.177%
2	5.690	479	485	488	rBV	3834954	4234246	76.44%	9.535%
3	6.678	646	653	656	rBV	3314942	4249097	76.71%	9.569%
4	7.054	714	717	721	rVB	1411765	1244199	22.46%	2.802%
5	7.625	807	814	817	rBV	2736471	2954681	53.34%	6.654%
6	8.342	931	936	939	rBV	2036237	1688754	30.49%	3.803%
7	9.425	1113	1120	1123	rBV	5760147	5539411	100.00%	12.475%
8	9.860	1187	1194	1196	rBV	56749	65783	1.19%	0.148%
9	10.107	1230	1236	1240	rBV	2330825	1993739	35.99%	4.490%
10	10.283	1260	1266	1274	rVB5	43433	75794	1.37%	0.171%
11	10.825	1354	1358	1361	rVB	2116435	1726915	31.18%	3.889%
12	10.901	1366	1371	1375	rBV	3896885	3839718	69.32%	8.647%
13	11.130	1407	1410	1415	rBV	265265	214598	3.87%	0.483%
14	11.201	1418	1422	1424	rBV	97697	81475	1.47%	0.183%
15	11.607	1487	1491	1494	rBV	2269414	1980513	35.75%	4.460%
16	11.701	1505	1507	1512	rVB2	78267	64214	1.16%	0.145%
17	12.119	1569	1578	1582	rBV	1263725	1443044	26.05%	3.250%
18	12.154	1582	1584	1592	rVB	136994	153398	2.77%	0.345%
19	12.824	1690	1698	1703	rBV	244864	302631	5.46%	0.682%
20	12.907	1703	1712	1723	rVB	524483	603466	10.89%	1.359%
21	13.060	1731	1738	1740	rBV	162567	176663	3.19%	0.398%
22	13.201	1757	1762	1765	rBV	5549627	5159893	93.15%	11.620%
23	13.413	1796	1798	1803	rBV	58990	60998	1.10%	0.137%
24	13.760	1852	1857	1859	rVB2	62093	75223	1.36%	0.169%
25	14.095	1910	1914	1928	rBV2	328688	751626	13.57%	1.693%
26	14.224	1932	1936	1939	rBV	167386	153392	2.77%	0.345%
27	14.265	1939	1943	1946	rBV	1477056	1320145	23.83%	2.973%
28	14.354	1954	1958	1963	rBV	73411	85999	1.55%	0.194%
29	14.407	1964	1967	1970	rVV	90405	72750	1.31%	0.164%
30	14.465	1973	1977	1983	rVB	202017	185274	3.34%	0.417%
31	14.718	2017	2020	2023	rBV	92260	85838	1.55%	0.193%
32	14.754	2023	2026	2040	rVB7	63654	185131	3.34%	0.417%
33	15.054	2074	2077	2084	rVB	66083	71952	1.30%	0.162%
34	15.142	2089	2092	2099	rVB2	72673	88401	1.60%	0.199%
35	15.218	2102	2105	2111	rVB2	56945	59291	1.07%	0.134%
36	15.365	2126	2130	2134	rBV	36758	63775	1.15%	0.144%

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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-BF013123.M
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37	15.430	2138	2141	2148	rVB	99985	118517	2.14%	0.267%
38	15.848	2206	2212	2224	rVB	765739	1065499	19.23%	2.399%
39	16.342	2292	2296	2305	rVB	70883	115545	2.09%	0.260%
40	16.483	2311	2320	2325	rBV9	25694	82052	1.48%	0.185%
41	17.689	2518	2525	2531	rBV5	54367	117411	2.12%	0.264%

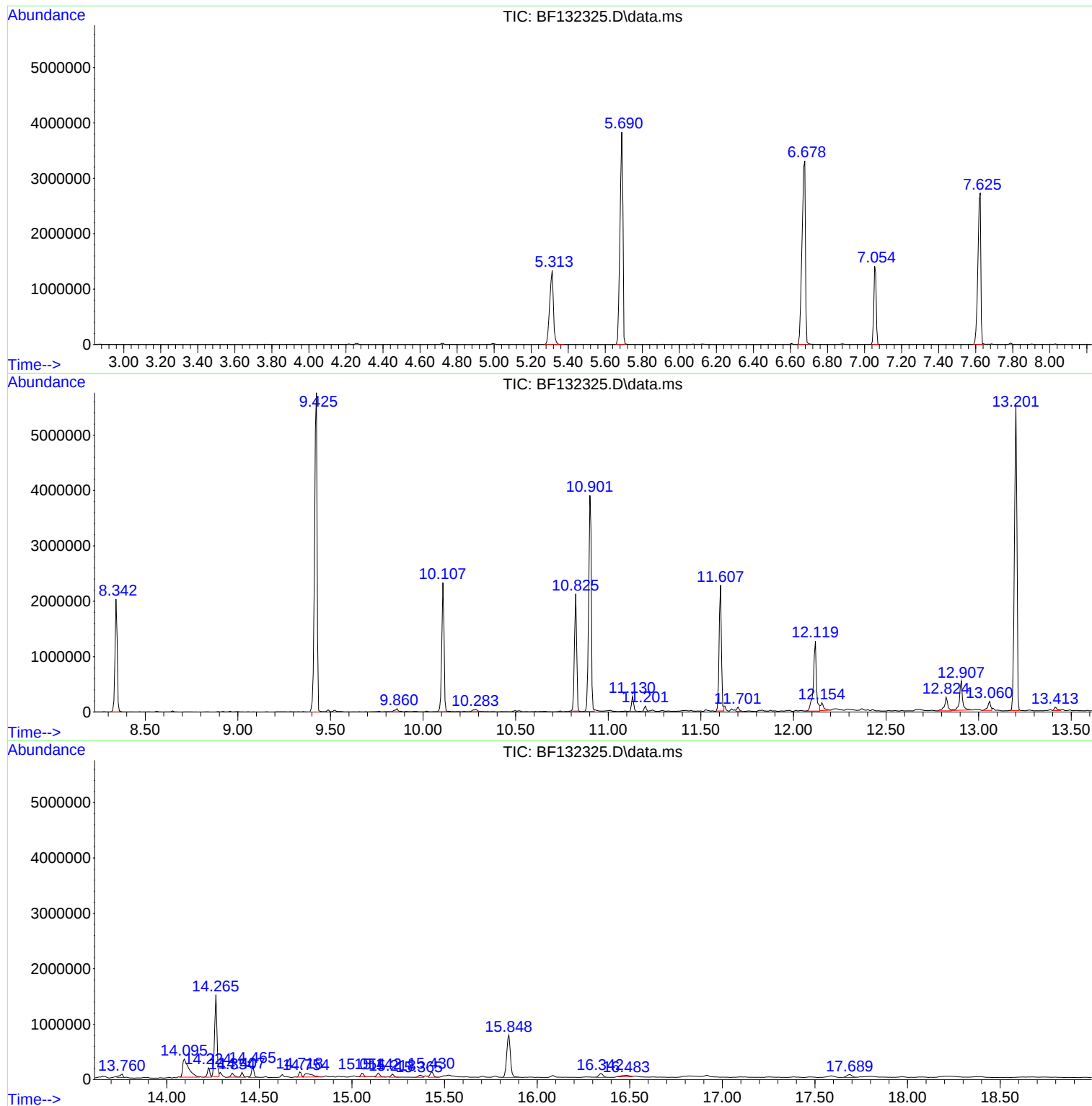
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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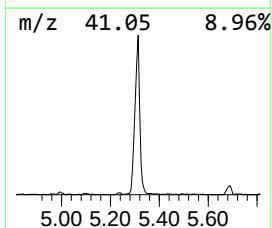
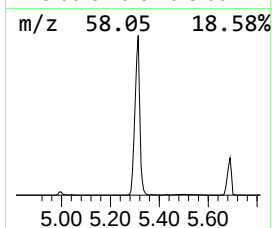
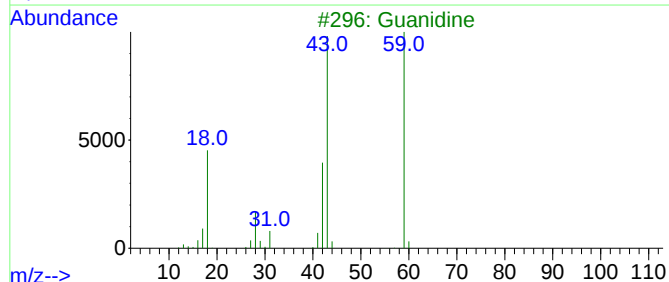
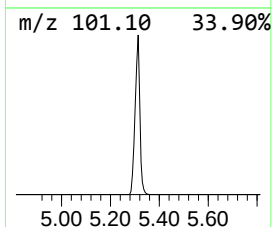
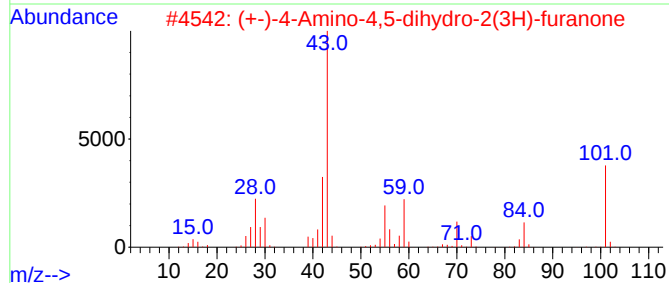
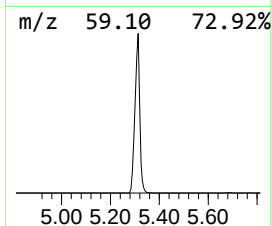
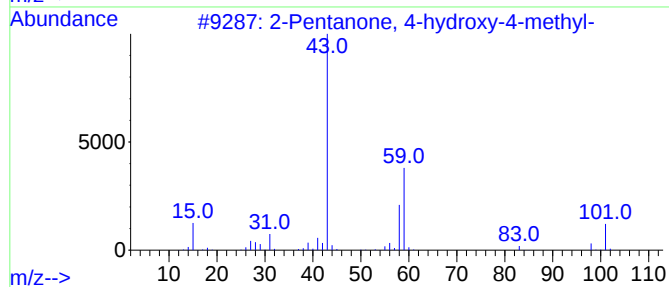
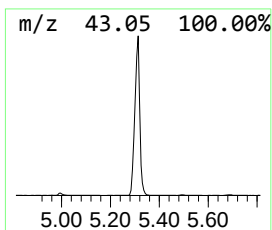
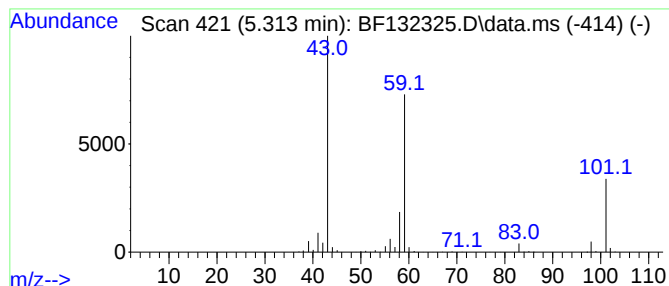
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.313	29.81 ng	1854730	1,4-Dichlorobenzene-d4	7.054

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47		
3	Guanidine	59	CH5N3	000113-00-8	43		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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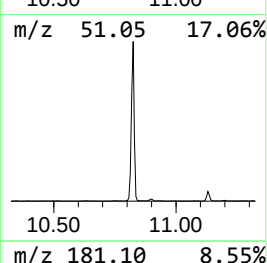
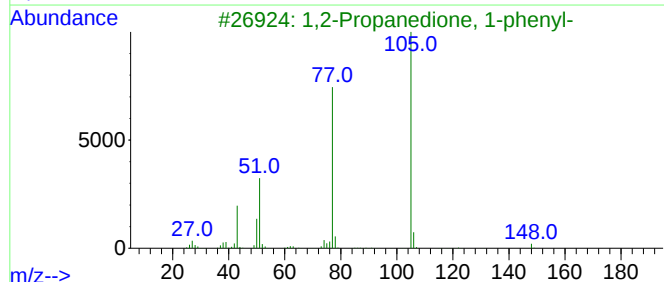
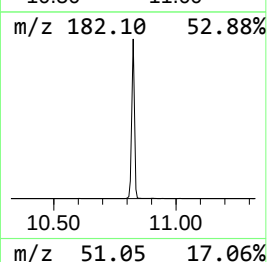
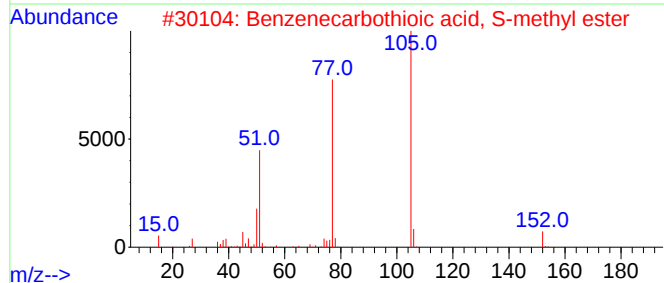
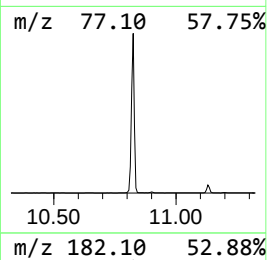
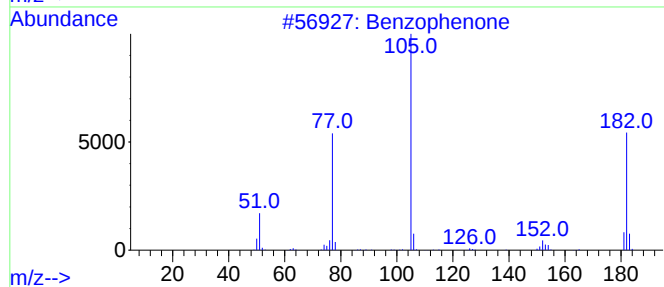
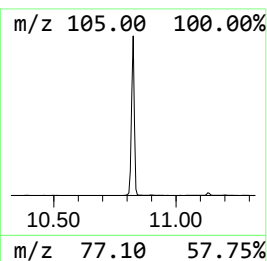
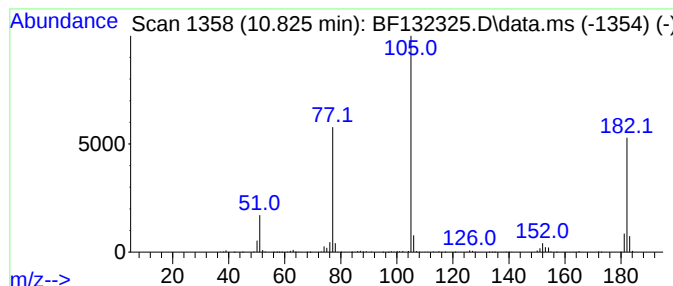
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.825	17.32 ng	1726920	Acenaphthene-d10	10.107

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	43
3			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	43
4			Methanone, (4-bromo-5-methyl-2-n...	357	C12H8BrNO3S2	1000274-00-2	43
5			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	43



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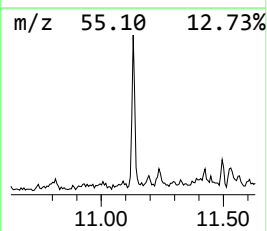
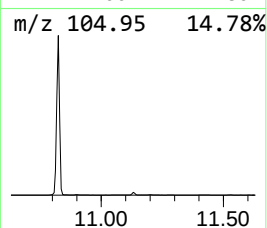
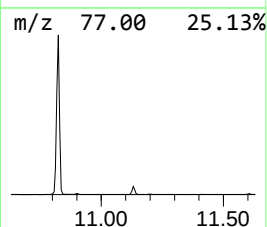
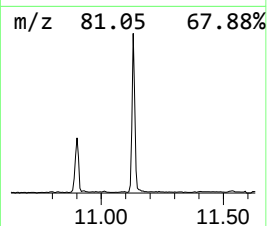
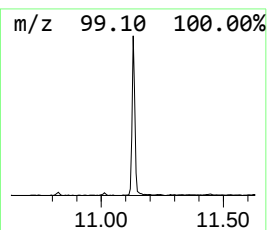
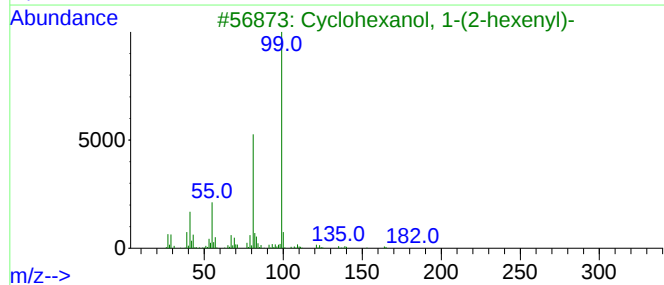
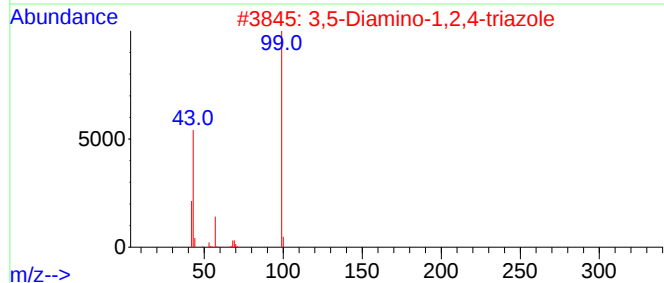
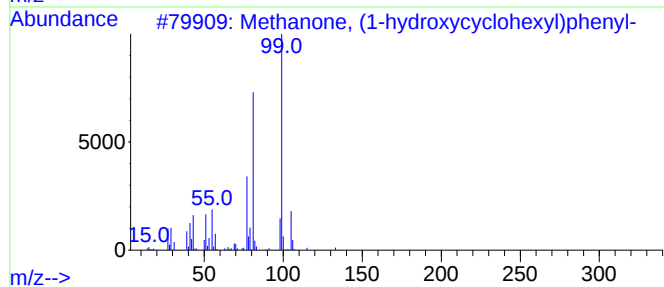
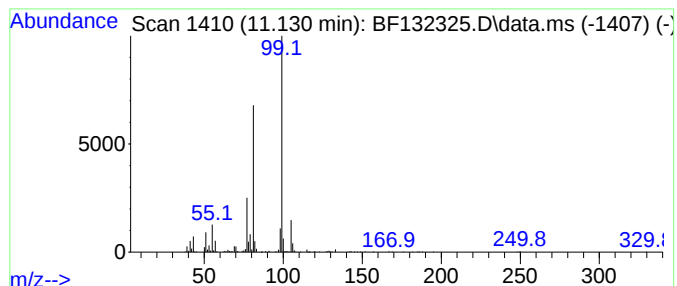
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Methanone, (1-hydroxycyclohexyl) Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.130	2.17 ng	214598	Phenanthrene-d10	11.607

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	83
2			3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	37
3			Cyclohexanol, 1-(2-hexenyl)-	182	C12H22O	054655-47-9	28
4			1,1'-Bicyclohexyl-1,1'-diol	198	C12H22O2	002888-11-1	28
5			Hexanoic acid, anhydride	214	C12H22O3	002051-49-2	25



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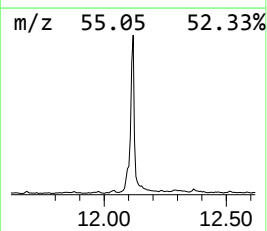
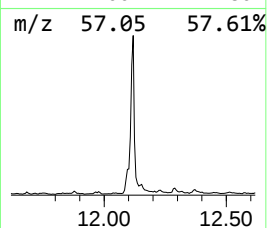
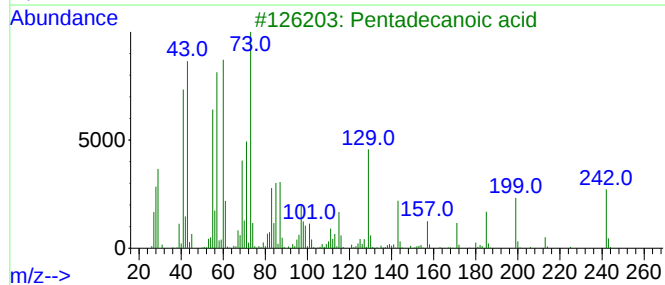
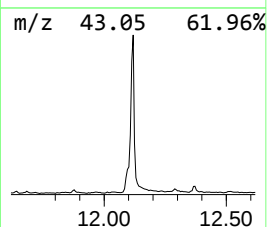
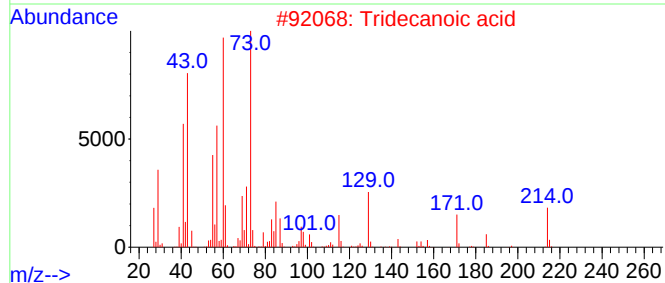
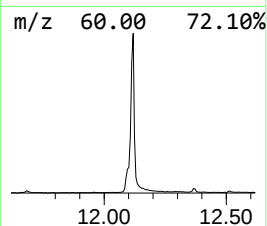
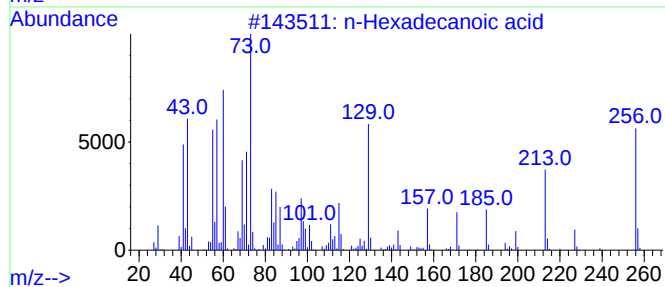
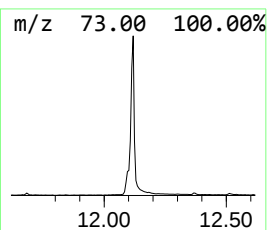
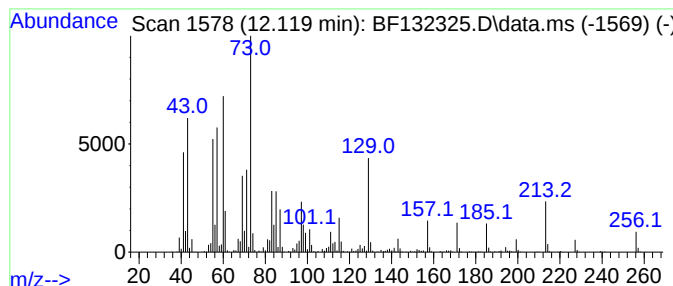
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.118	14.57 ng	1443040	Phenanthrene-d10	11.607

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			n-Decanoic acid	172	C10H20O2	000334-48-5	62
5			Dodecanoic acid	200	C12H24O2	000143-07-7	49



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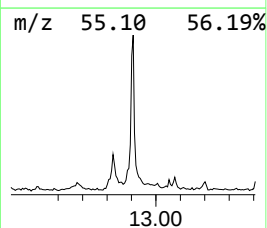
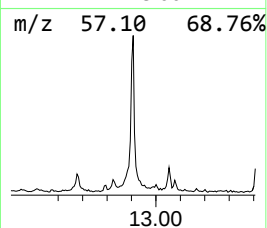
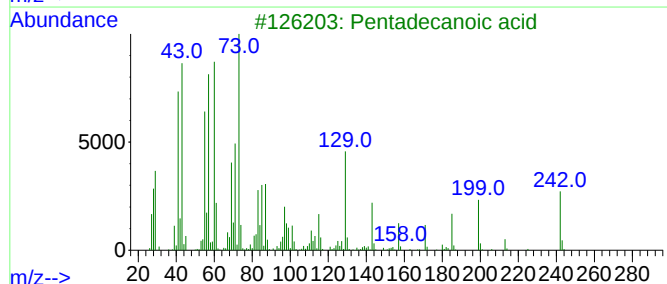
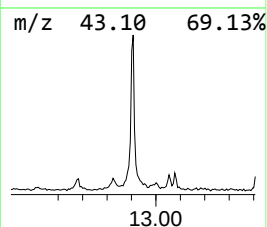
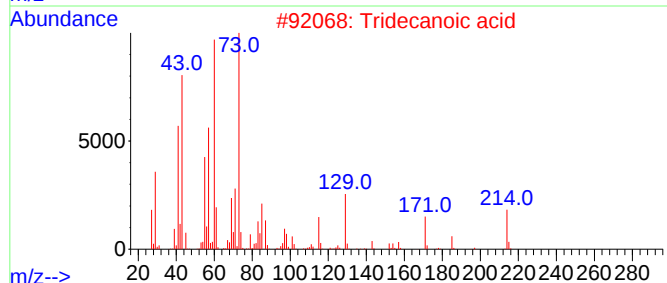
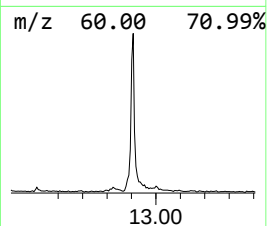
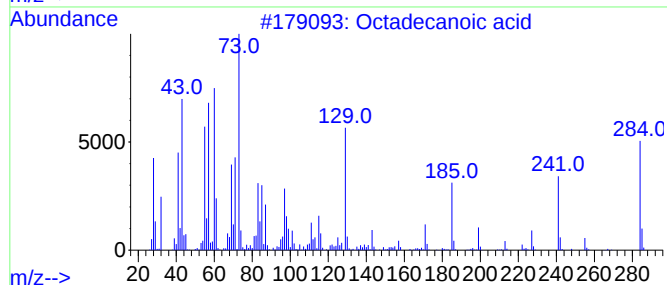
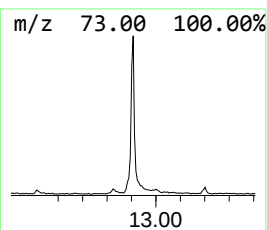
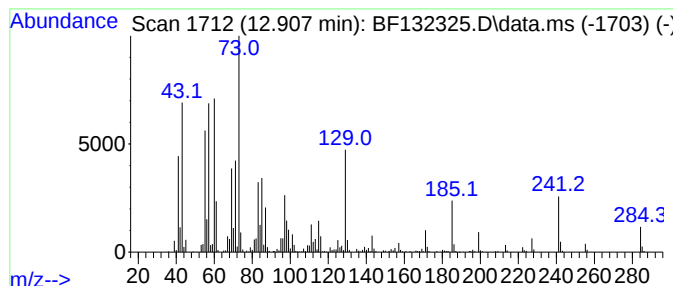
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
12.907	6.09 ng	603466	Phenanthrene-d10	11.607

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	62
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4			n-Decanoic acid	172	C10H20O2	000334-48-5	58
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020323\
Data File : BF132325.D
Acq On : 03 Feb 2023 16:59
Operator : CG\JU
Sample : 01371-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
4-RAMP-E

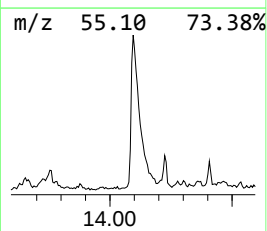
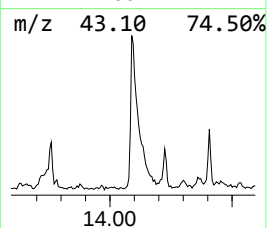
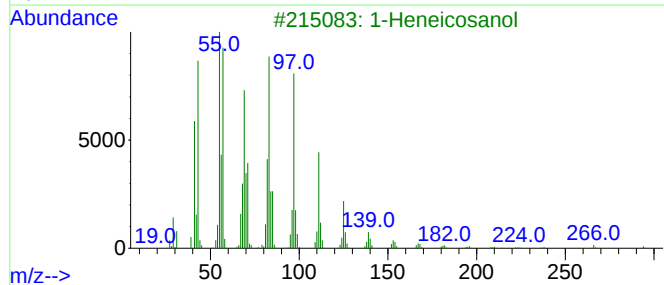
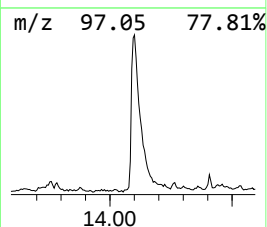
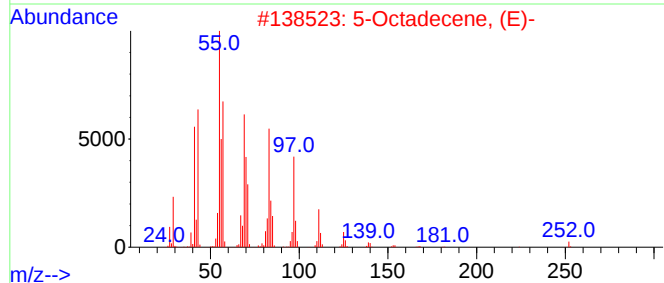
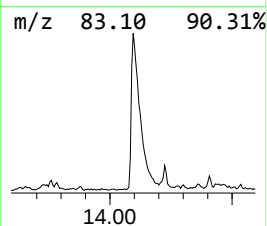
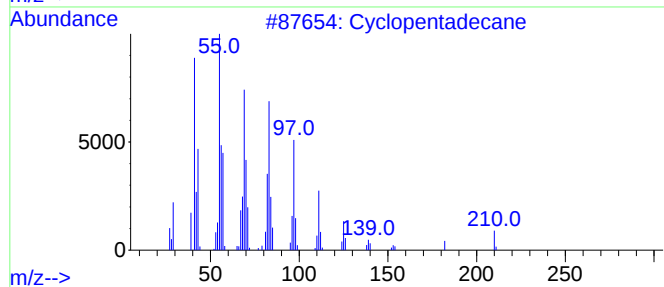
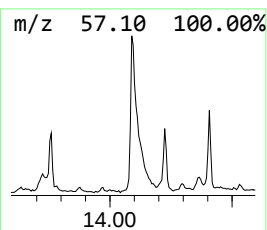
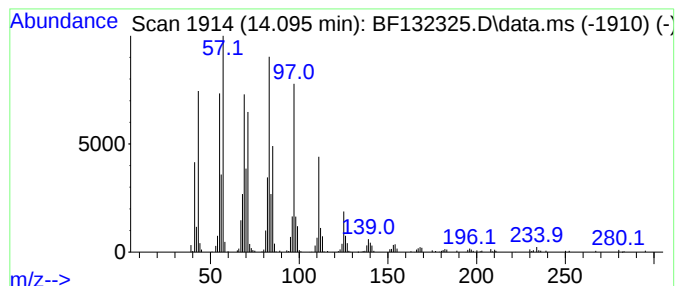
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.095	11.39 ng	751626	Chrysene-d12	14.265

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	94
2			5-Octadecene, (E)-	252	C18H36	007206-21-5	93
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020323\
Data File : BF132325.D
Acq On : 03 Feb 2023 16:59
Operator : CG\JU
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Misc :
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4-RAMP-E

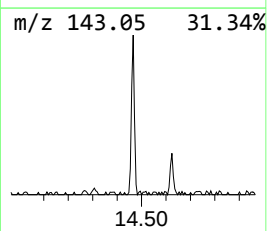
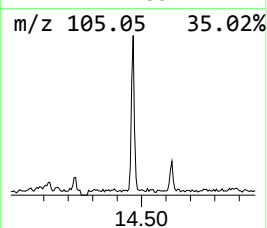
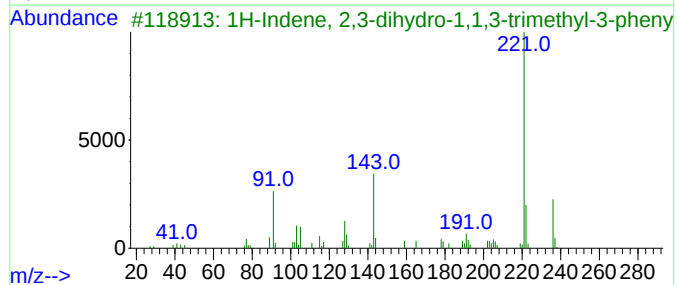
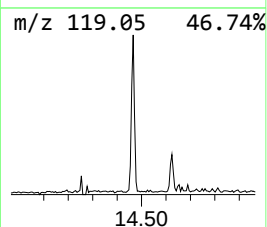
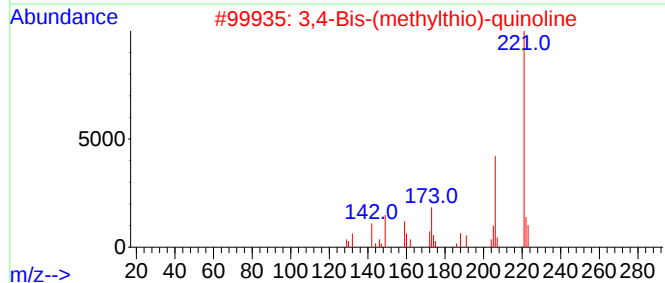
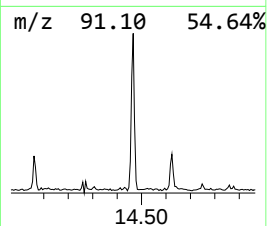
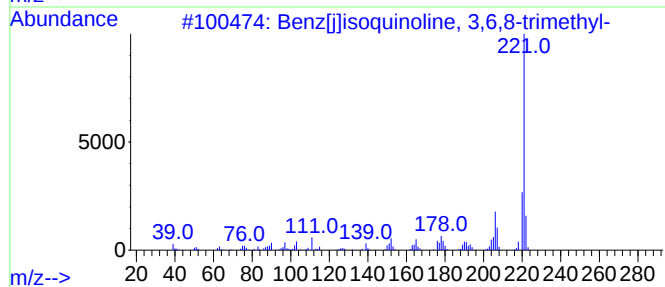
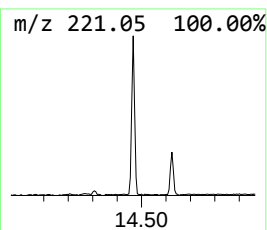
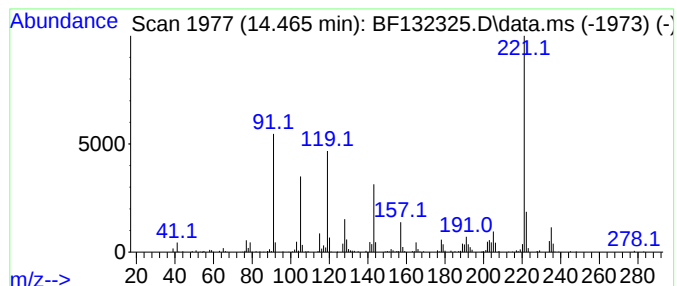
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benz[j]isoquinoline, 3,6,8-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.465	2.81 ng	185274	Chrysene-d12	14.265

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benz[j]isoquinoline, 3,6,8-trime...	221	C16H15N	061171-16-2	50
2			3,4-Bis-(methylthio)-quinoline	221	C11H11NS2	074579-34-3	50
3			1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	50
4			Indole, 5-(4-methylphenyl)-N-met...	221	C16H15N	1000380-54-7	46
5			3-Amino-4,6-dimethylthieno[2,3-b...	221	C10H11N3OS	067795-42-0	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020323\
Data File : BF132325.D
Acq On : 03 Feb 2023 16:59
Operator : CG\JU
Sample : 01371-04
Misc :
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Instrument :
BNA_F
ClientSampleId :
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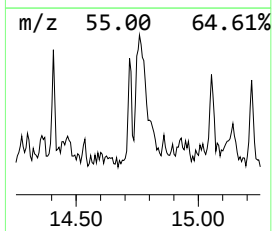
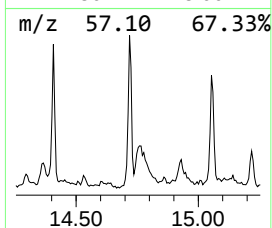
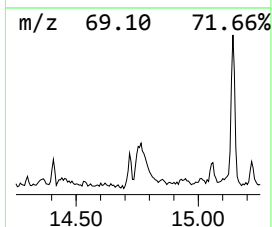
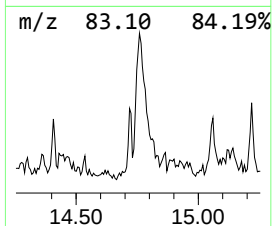
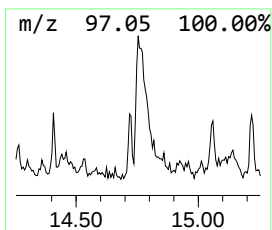
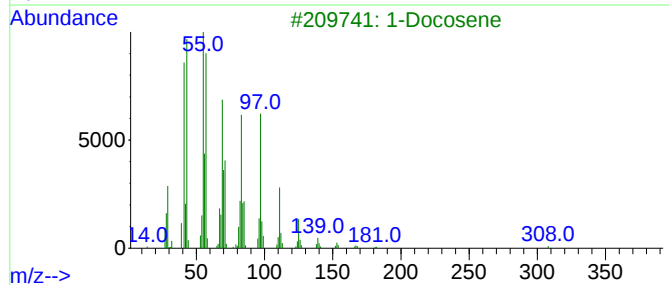
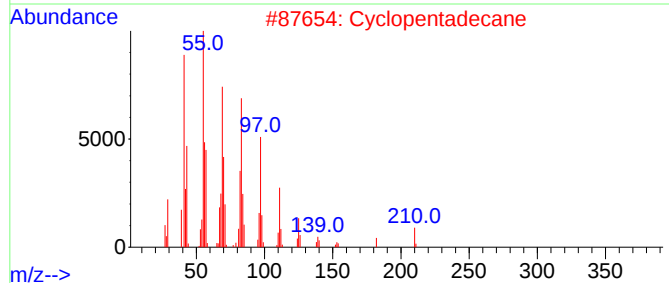
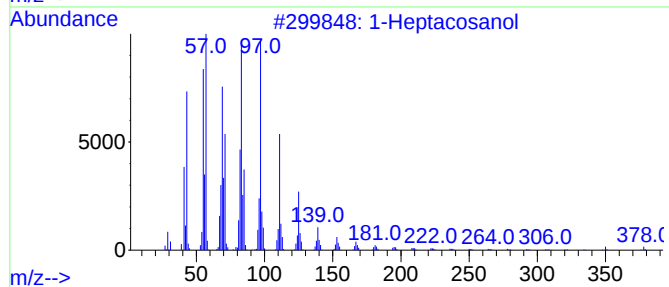
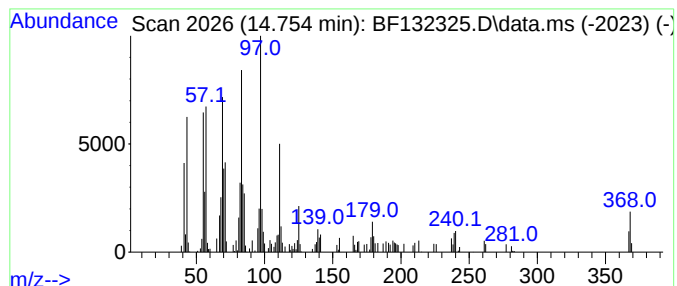
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.754	2.80 ng	185131	Chrysene-d12	14.265

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptacosanol	396	C27H56O	002004-39-9	93
2		Cyclopentadecane	210	C15H30	000295-48-7	92
3		1-Docosene	308	C22H44	001599-67-3	90
4		1-Heneicosanol	312	C21H44O	015594-90-8	90
5		Cyclotetradecane	196	C14H28	000295-17-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020323\
Data File : BF132325.D
Acq On : 03 Feb 2023 16:59
Operator : CG\JU
Sample : 01371-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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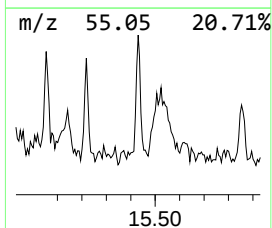
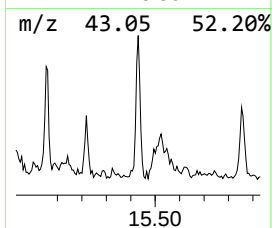
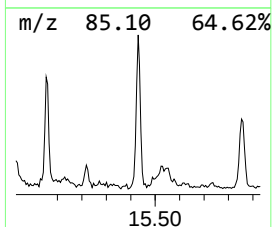
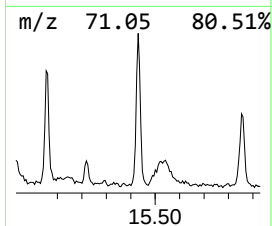
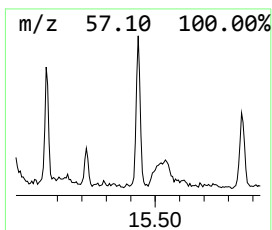
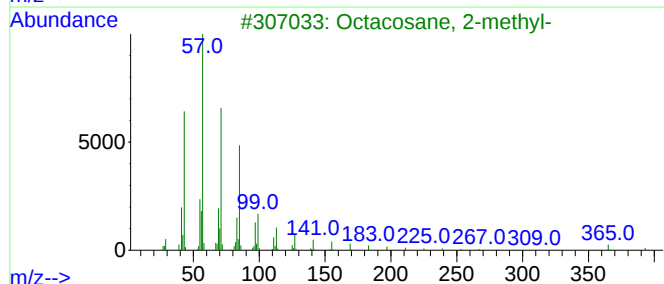
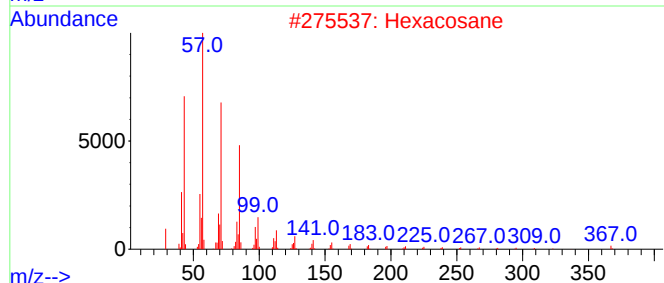
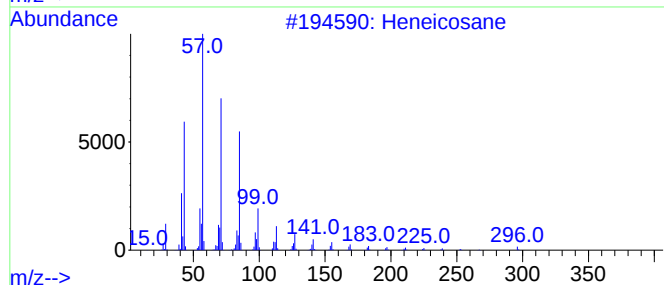
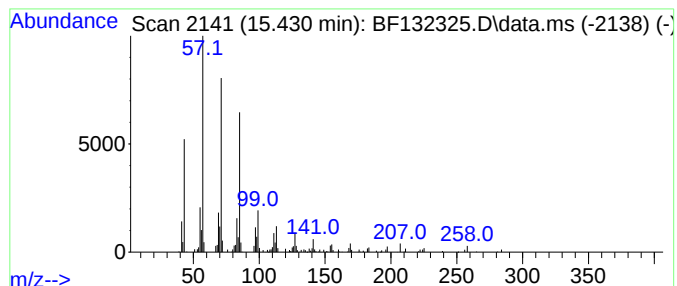
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.430	2.22 ng	118517	Perylene-d12	15.848

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4			Triacontane	422	C30H62	000638-68-6	91
5			Heptacosane	380	C27H56	000593-49-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020323\
Data File : BF132325.D
Acq On : 03 Feb 2023 16:59
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Misc :
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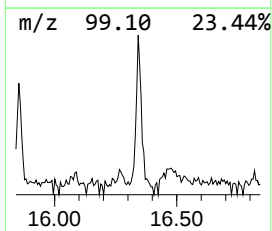
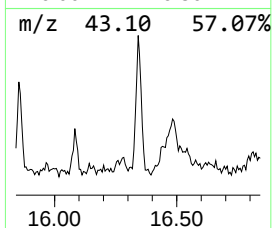
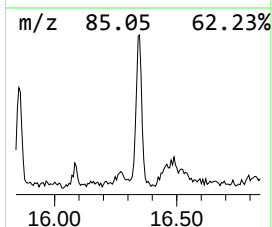
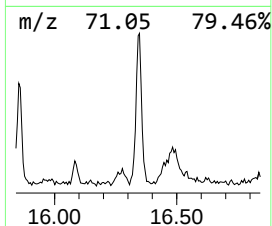
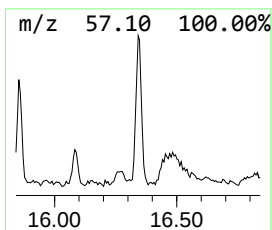
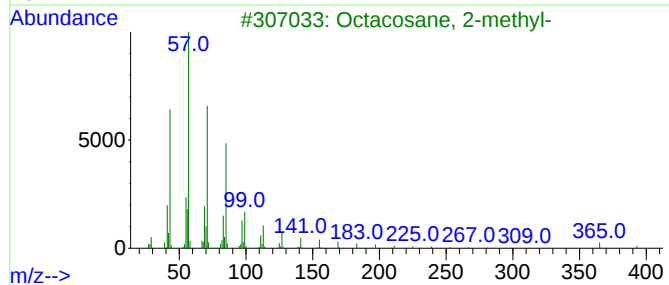
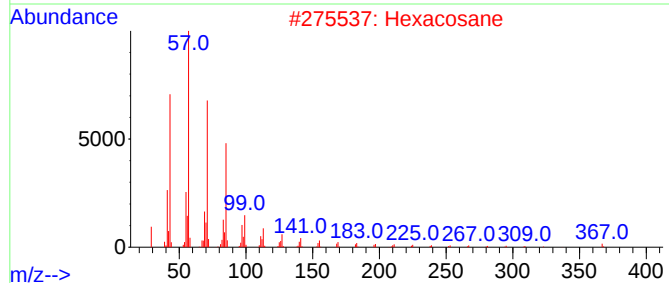
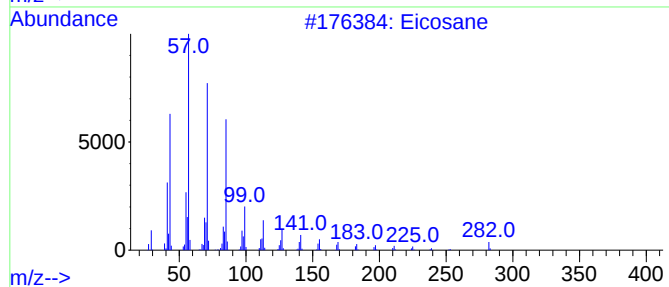
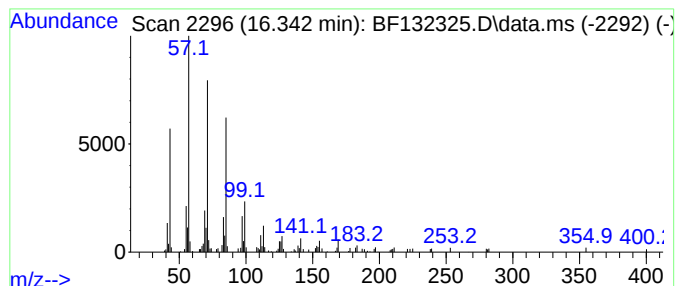
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.342	2.17 ng	115545	Perylene-d12	15.848	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020323\
Data File : BF132325.D
Acq On : 03 Feb 2023 16:59
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Sample : 01371-04
Misc :
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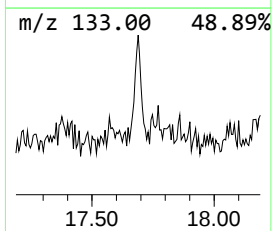
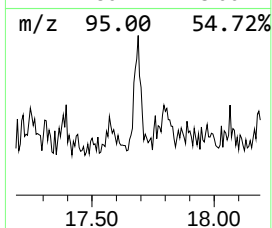
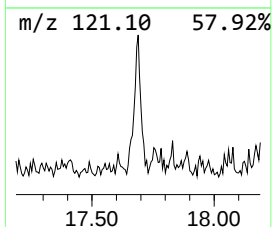
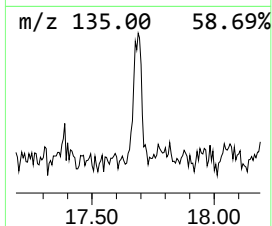
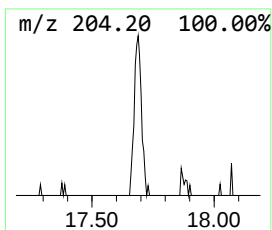
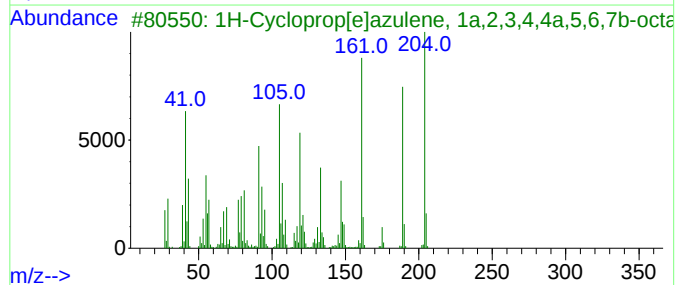
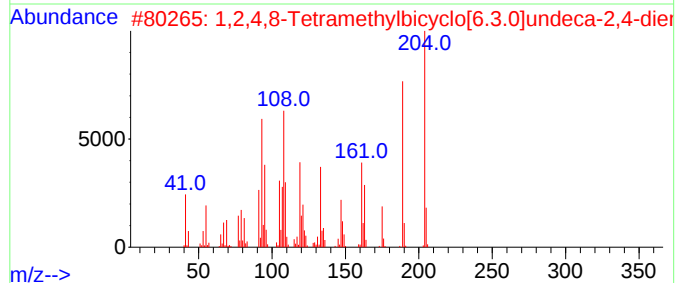
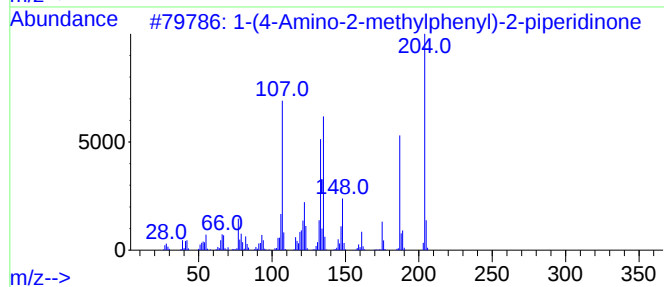
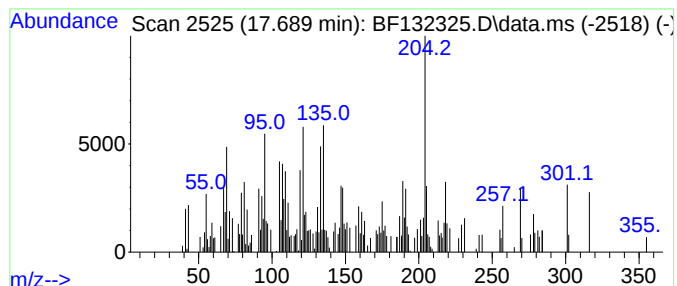
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-(4-Amino-2-methylphenyl)-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.689	2.20 ng	117411	Perylene-d12	15.848

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(4-Amino-2-methylphenyl)-2-pip...	204	C12H16N2O	443999-53-9	60		
2	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	55		
3	1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	45		
4	Aciphyllene	204	C15H24	087745-31-1	43		
5	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	42		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020323\
Data File : BF132325.D
Acq On : 03 Feb 2023 16:59
Operator : CG\JU
Sample : 01371-04
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.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
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Benzophenone	10.825	17.3	ng	1726920	3	10.107	1993740	20.0
Methanone, (1-h...	11.130	2.2	ng	214598	4	11.607	1980510	20.0
n-Hexadecanoic ...	12.118	14.6	ng	1443040	4	11.607	1980510	20.0
Octadecanoic acid	12.907	6.1	ng	603466	4	11.607	1980510	20.0
Cyclopentadecane	14.095	11.4	ng	751626	5	14.265	1320150	20.0
Benz[j]isoquino...	14.465	2.8	ng	185274	5	14.265	1320150	20.0
1-Heptacosanol	14.754	2.8	ng	185131	5	14.265	1320150	20.0
Heneicosane	15.430	2.2	ng	118517	6	15.848	1065500	20.0
Eicosane	16.342	2.2	ng	115545	6	15.848	1065500	20.0
1-(4-Amino-2-me...	17.689	2.2	ng	117411	6	15.848	1065500	20.0