

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050923\
 Data File : BF133315.D
 Acq On : 09 May 2023 14:00
 Operator : CG\JU
 Sample : 02665-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TR-612-COMP-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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133315.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.263	366	370	377	rVB	59381	75970	1.47%	0.175%
2	4.916	475	481	490	rBV	1606720	2171194	42.15%	5.010%
3	5.340	548	553	556	rBV	4480341	4439109	86.18%	10.242%
4	5.728	615	619	626	rVB	141878	118546	2.30%	0.274%
5	6.363	722	727	730	rBV	4161114	4592590	89.16%	10.596%
6	6.716	784	787	791	rBV	1446624	1267495	24.61%	2.924%
7	7.287	879	884	887	rBV	3426164	2957285	57.41%	6.823%
8	8.004	1002	1006	1009	rBV	2262258	1707464	33.15%	3.940%
9	9.081	1185	1189	1192	rBV	5747448	5022414	97.50%	11.588%
10	9.757	1300	1304	1307	rBV	2358191	1950189	37.86%	4.500%
11	10.469	1421	1425	1428	rBV	1623915	1300648	25.25%	3.001%
12	10.545	1433	1438	1441	rBV	3273837	2932939	56.94%	6.767%
13	10.775	1473	1477	1482	rBV	299702	251086	4.87%	0.579%
14	10.863	1488	1492	1496	rBV	266689	241322	4.68%	0.557%
15	11.157	1539	1542	1546	rVB	146935	107823	2.09%	0.249%
16	11.233	1552	1555	1558	rBV	2161718	2026031	39.33%	4.675%
17	11.257	1558	1559	1564	rVB2	118362	86691	1.68%	0.200%
18	11.775	1637	1647	1656	rBV4	402456	721539	14.01%	1.665%
19	12.339	1736	1743	1746	rBV5	48656	102938	2.00%	0.238%
20	12.445	1758	1761	1764	rBV	241399	188402	3.66%	0.435%
21	12.557	1774	1780	1790	rVB	544666	976896	18.96%	2.254%
22	12.674	1794	1800	1803	rVB	204436	219078	4.25%	0.505%
23	12.827	1821	1826	1829	rBV	5362741	5151237	100.00%	11.885%
24	13.063	1863	1866	1869	rBV2	74993	72441	1.41%	0.167%
25	13.733	1975	1980	1981	rBV2	77842	88071	1.71%	0.203%
26	13.763	1981	1985	1996	rVV3	187134	582849	11.31%	1.345%
27	13.868	1999	2003	2006	rVV	1576921	1655337	32.13%	3.819%
28	13.892	2006	2007	2014	rVV	106627	98698	1.92%	0.228%
29	13.968	2016	2020	2025	rVV3	46261	60269	1.17%	0.139%
30	14.051	2030	2034	2040	rVB	66511	80968	1.57%	0.187%
31	14.351	2082	2085	2088	rVB	80268	77750	1.51%	0.179%
32	14.627	2129	2132	2134	rBV	156036	162802	3.16%	0.376%
33	14.651	2134	2136	2144	rVB	138582	171016	3.32%	0.395%
34	14.886	2172	2176	2179	rBV	64601	94751	1.84%	0.219%
35	14.968	2187	2190	2200	rVB2	93902	136761	2.65%	0.316%
36	15.227	2230	2234	2240	rBV	52676	63354	1.23%	0.146%

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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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.286	2240	2244	2249	rVV	937626	1140538	22.14%	2.632%
38	15.327	2249	2251	2256	rVB	76256	98679	1.92%	0.228%
39	15.739	2317	2321	2328	rVB	53609	79594	1.55%	0.184%
40	16.215	2398	2402	2411	rVB6	29552	68189	1.32%	0.157%

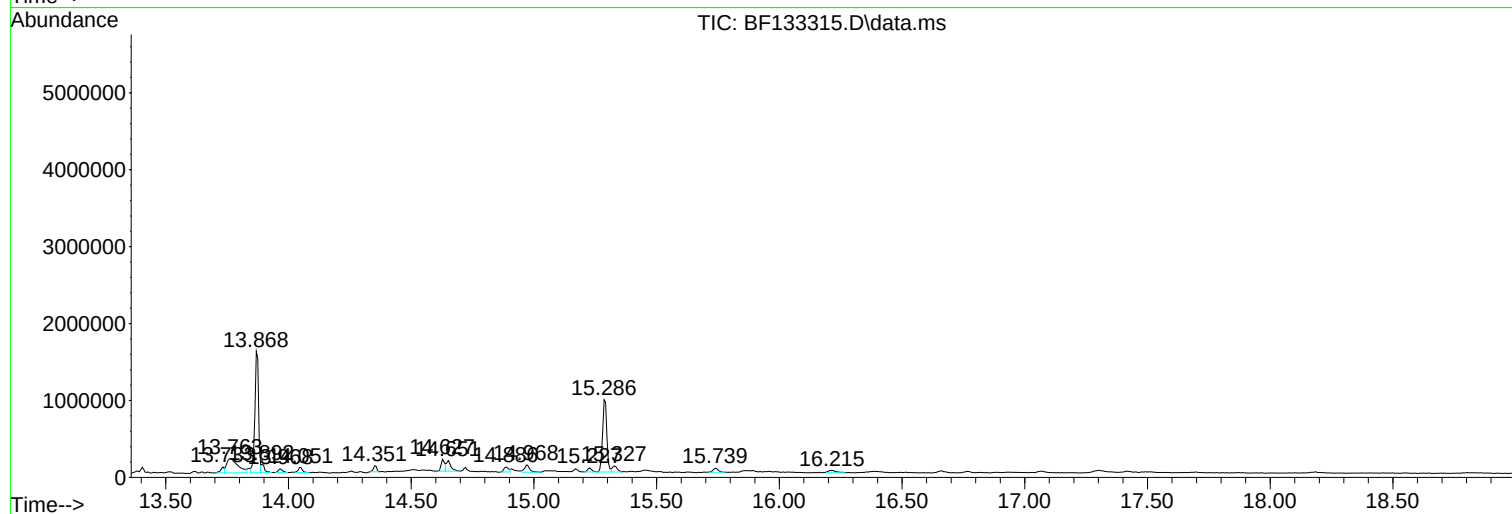
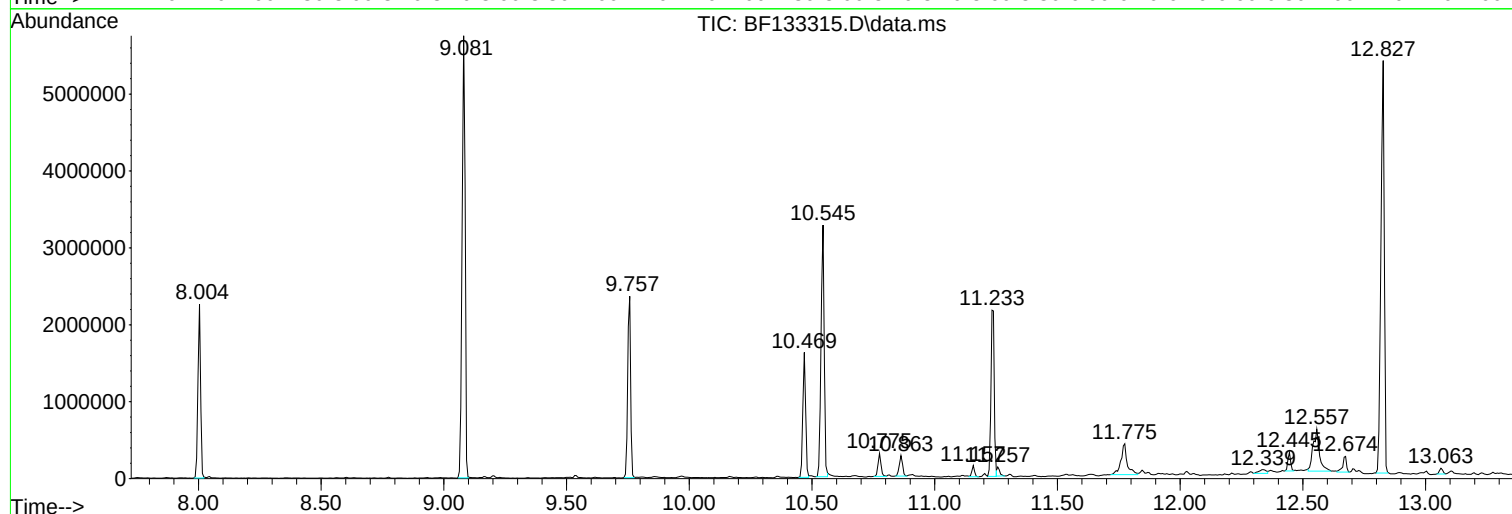
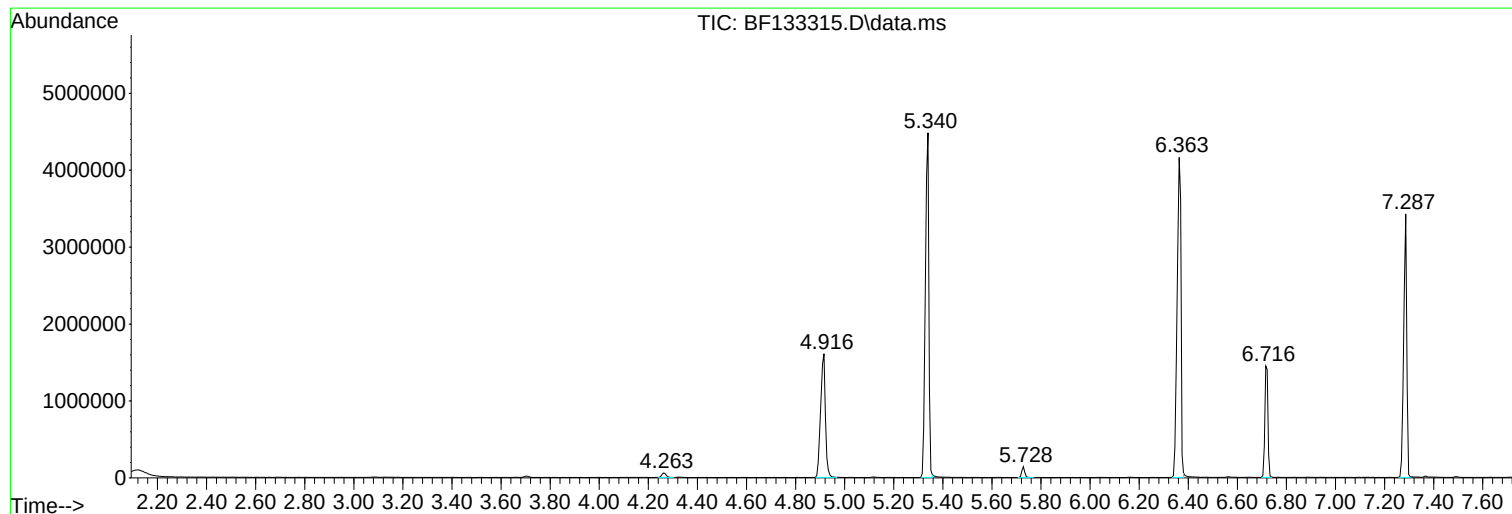
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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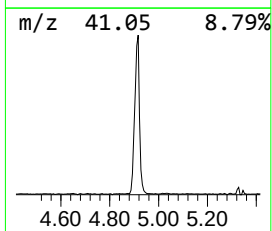
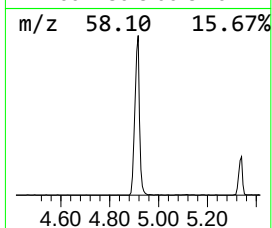
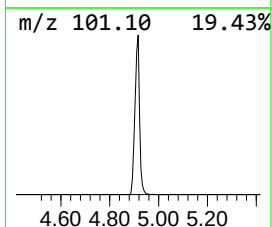
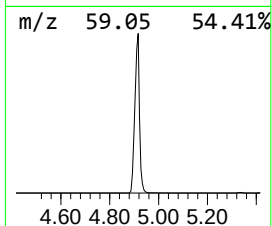
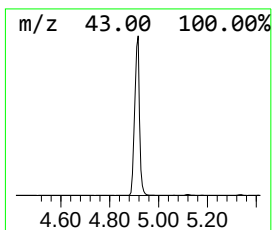
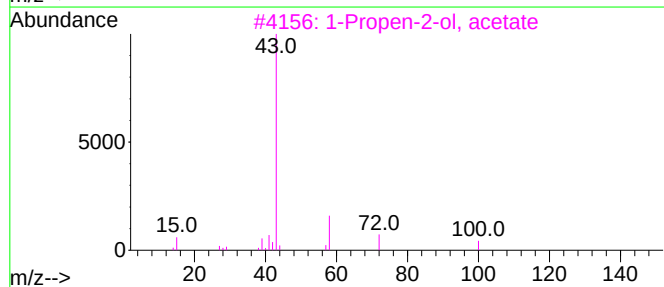
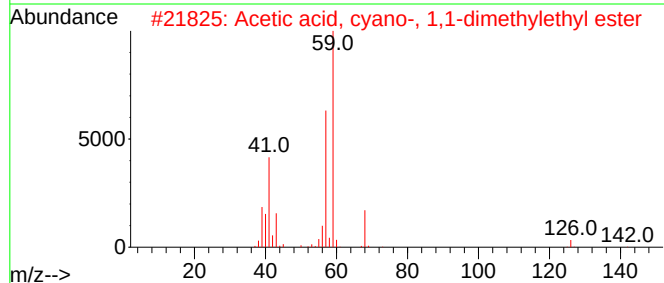
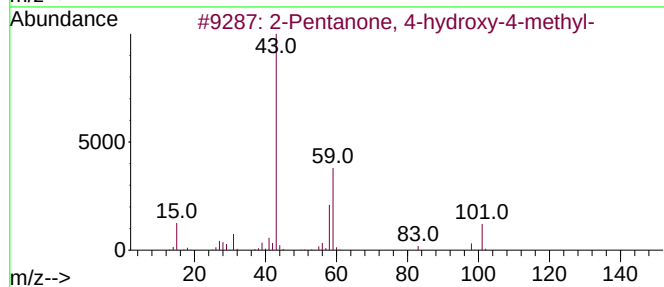
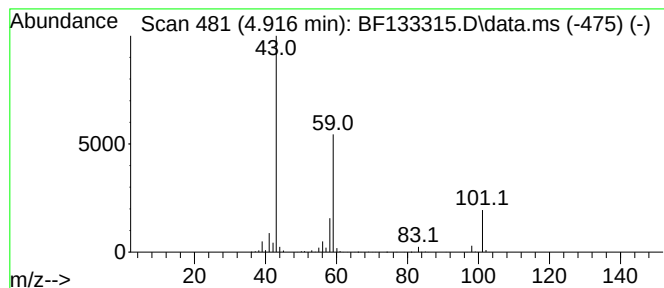
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.916	34.26 ng	2171190	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	50		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9		



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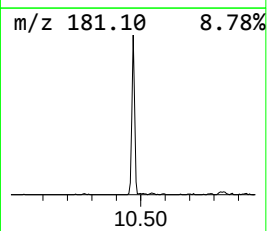
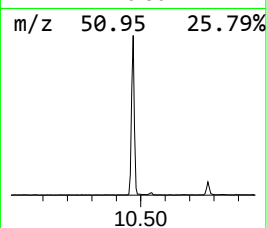
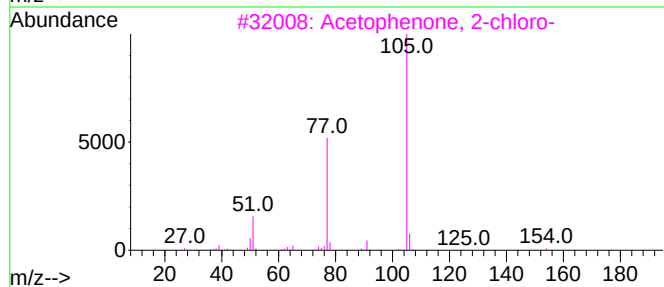
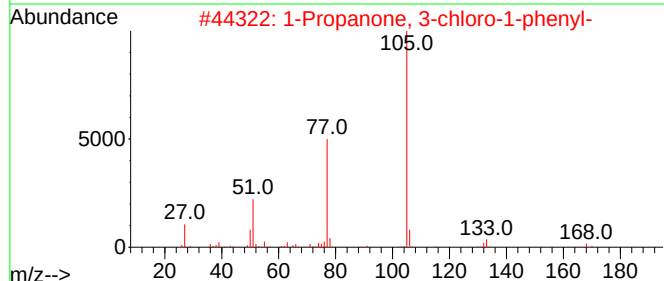
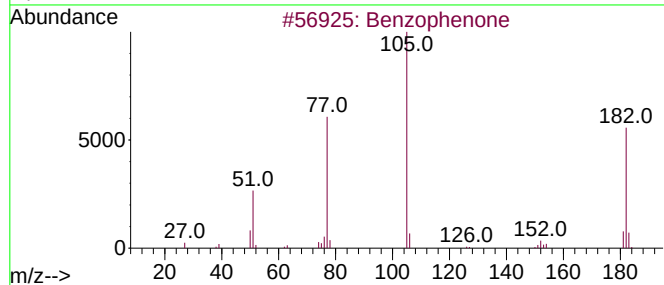
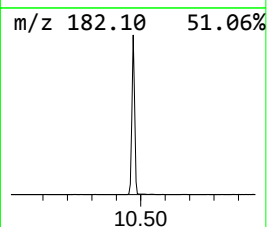
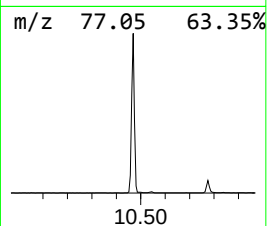
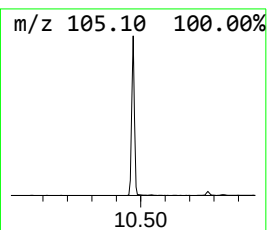
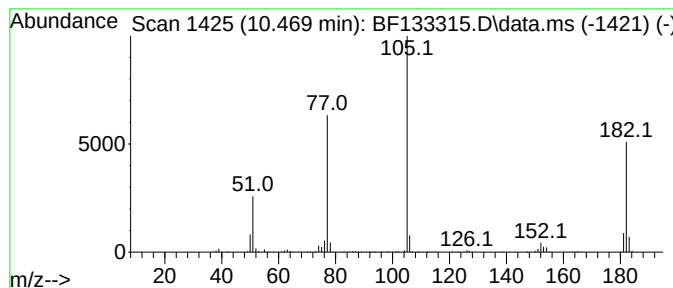
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	13.34 ng	1300650	Acenaphthene-d10	9.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
4			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
5			Vinyl benzoate	148	C9H8O2	000769-78-8	47



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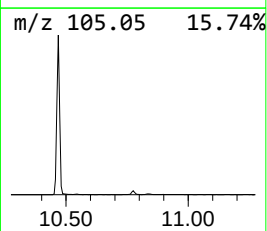
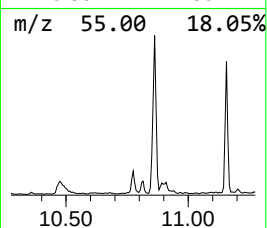
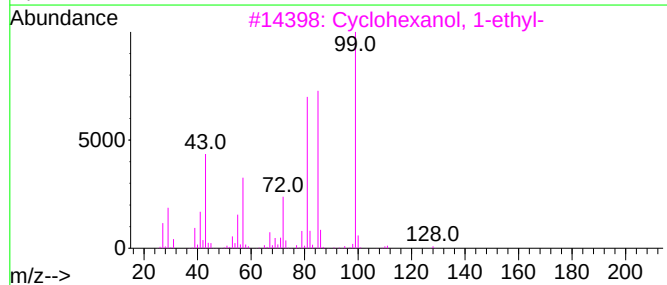
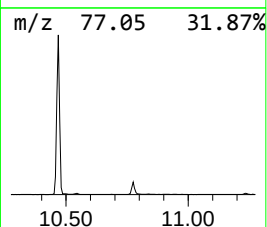
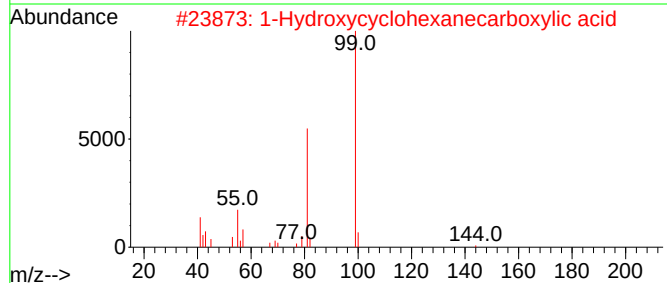
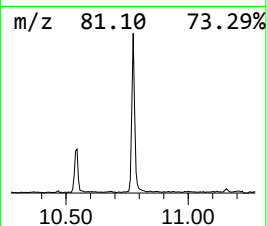
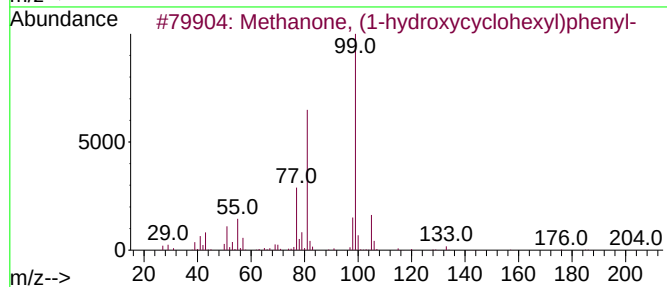
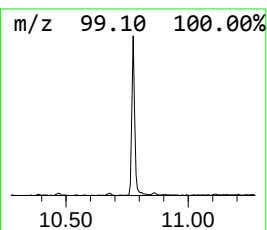
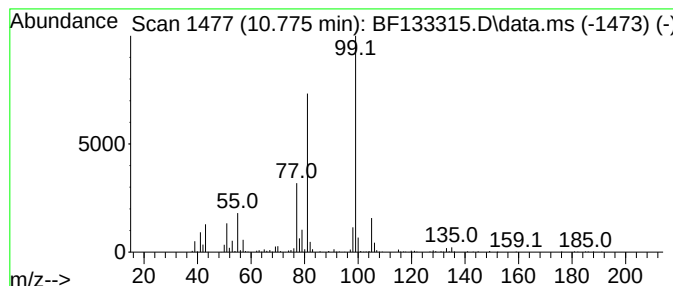
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Methanone, (1-hydroxycyclohexyl) Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.775	2.48 ng	251086	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	91
2			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	59
3			Cyclohexanol, 1-ethyl-	128	C8H16O	001940-18-7	59
4			3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	59
5			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	50



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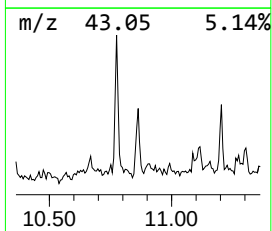
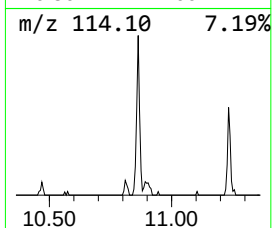
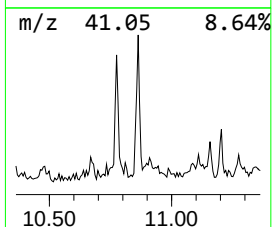
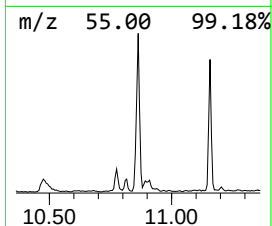
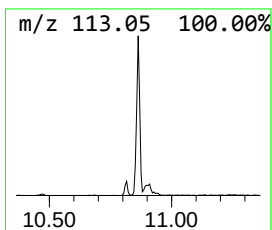
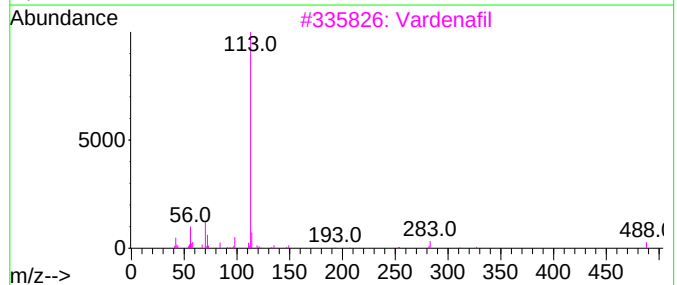
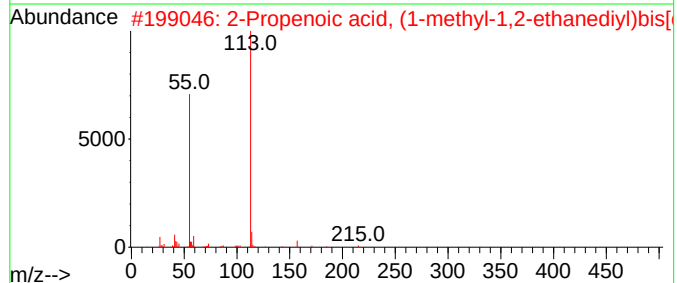
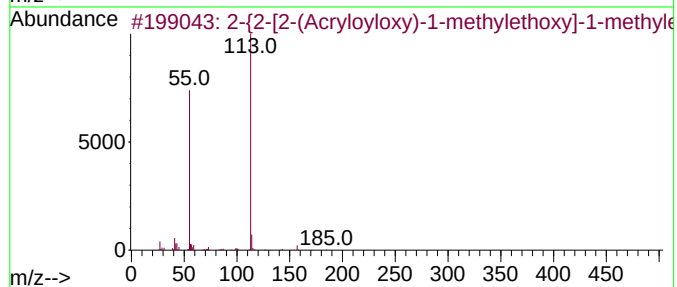
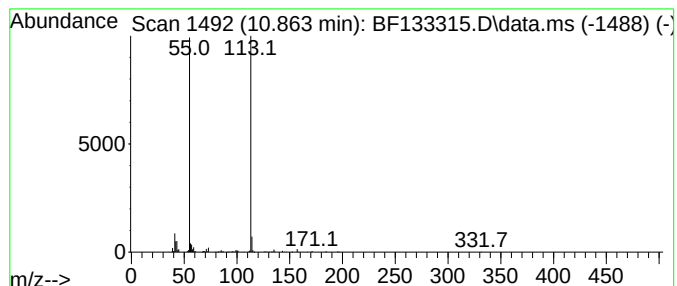
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 2-{2-[2-(Acryloyloxy)-1-met... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.863	2.38 ng	241322	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2	-{2-[2-(Acryloyloxy)-1-methylet...	300	C15H24O6	094120-00-0	83	
2	2	Propenoic acid, (1-methyl-1,2-...	300	C15H24O6	042978-66-5	83	
3	Vardenafil	488	C23H32N6O4S	224785-90-4	38		
4	Heptanoic acid, anhydride	242	C14H26O3	000626-27-7	38		
5	2H-Pyrrol-2-one, 1,5-dihydro-4-m...	113	C5H7NO2	069778-83-2	9		



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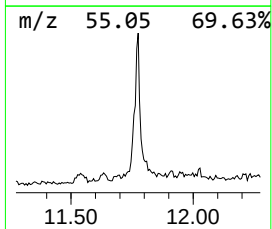
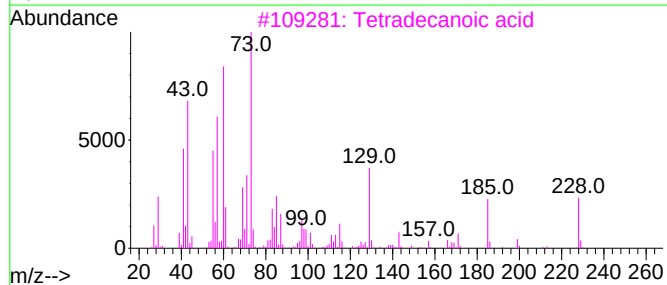
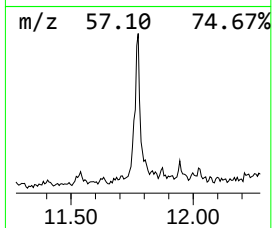
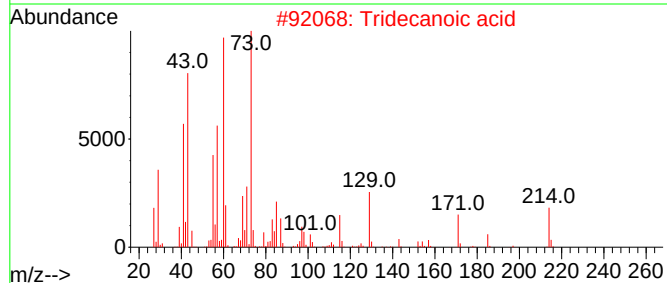
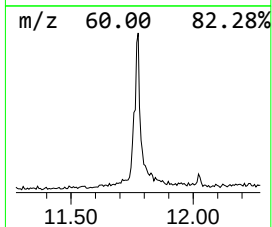
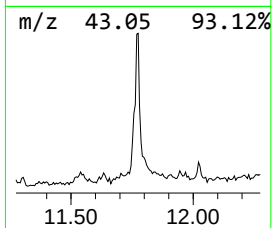
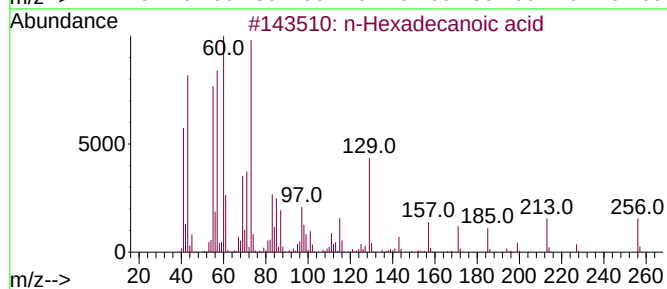
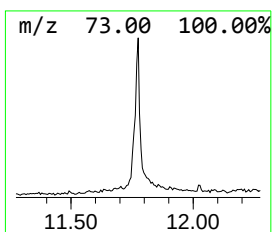
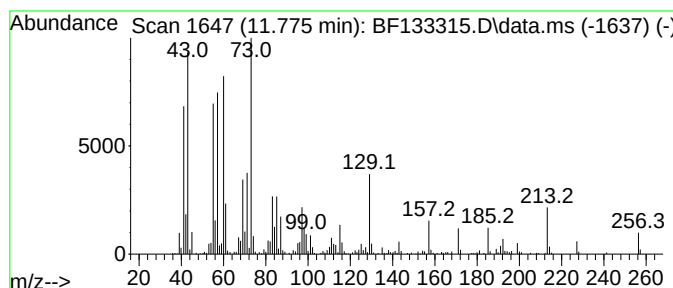
Instrument :
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ClientSampleId :
TR-612-COMP-01

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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 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.775	7.12 ng	721539	Phenanthrene-d10	11.239	
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	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Dodecanoic acid	200	C12H24O2	000143-07-7	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050923\
Data File : BF133315.D
Acq On : 09 May 2023 14:00
Operator : CG\JU
Sample : 02665-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-612-COMP-01

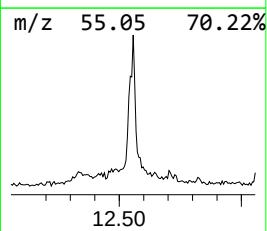
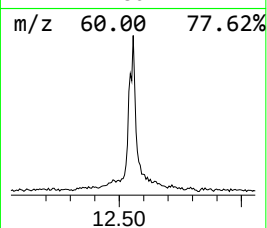
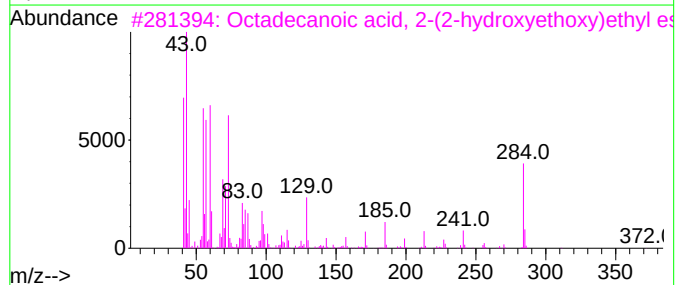
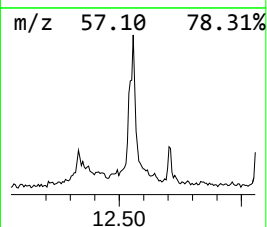
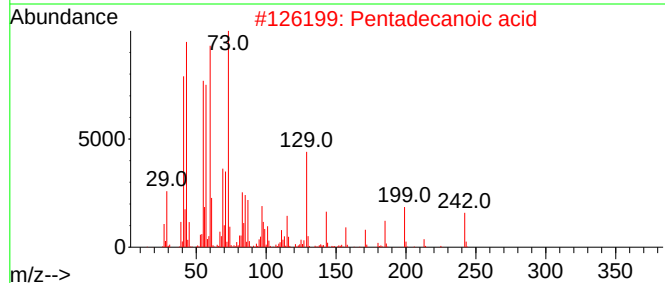
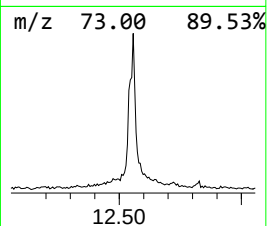
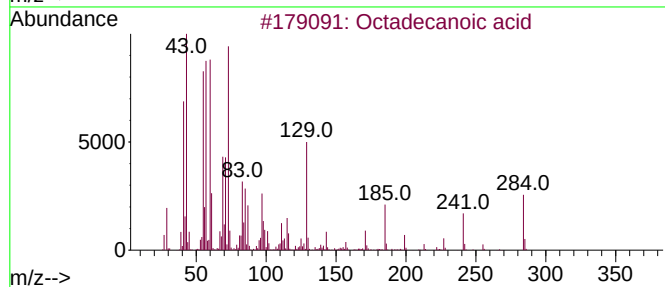
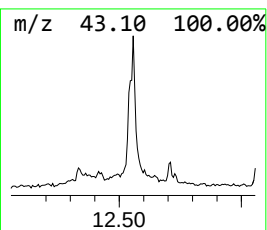
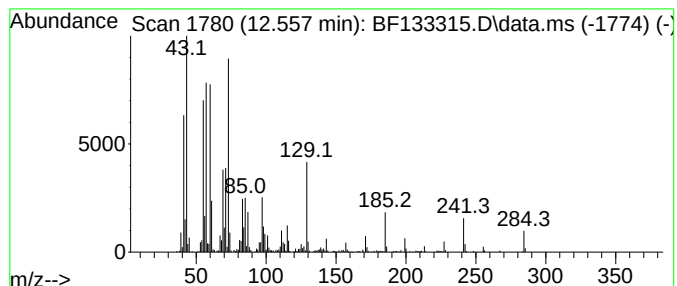
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.557	11.80 ng	976896	Chrysene-d12	13.868

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	91
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050923\
Data File : BF133315.D
Acq On : 09 May 2023 14:00
Operator : CG\JU
Sample : 02665-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-612-COMP-01

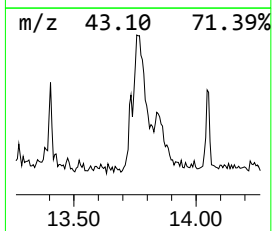
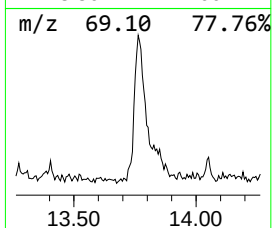
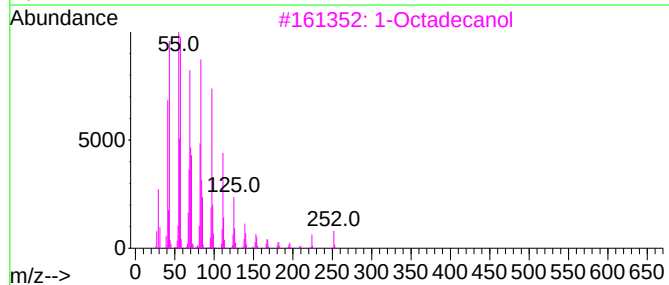
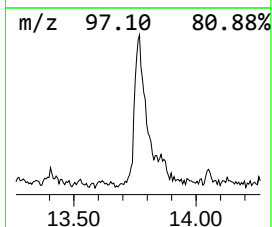
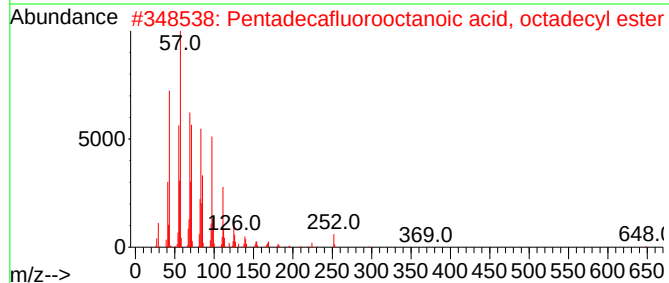
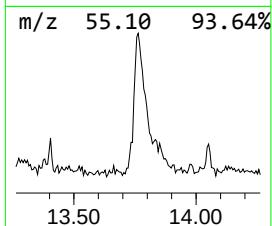
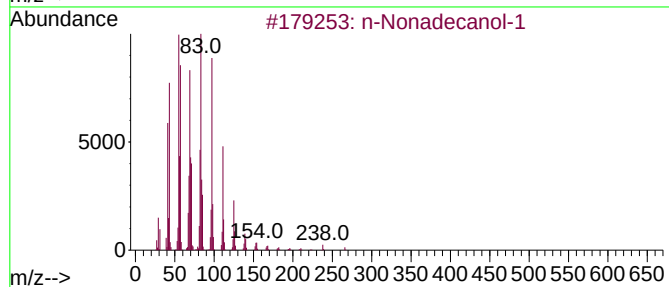
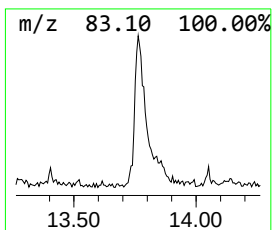
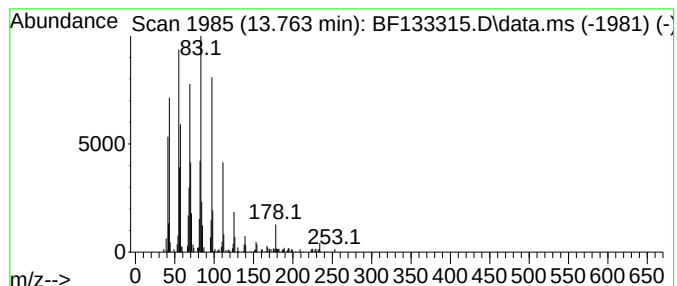
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.763	7.04 ng	582849	Chrysene-d12	13.868

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Nonadecanol-1	284	C19H40O	001454-84-8	90
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	80
3			1-Octadecanol	270	C18H38O	000112-92-5	72
4			Cyclooctane, methyl-	126	C9H18	001502-38-1	60
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050923\
Data File : BF133315.D
Acq On : 09 May 2023 14:00
Operator : CG\JU
Sample : 02665-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TR-612-COMP-01

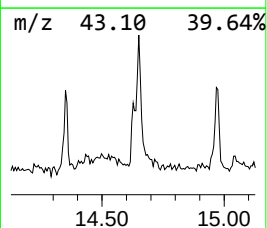
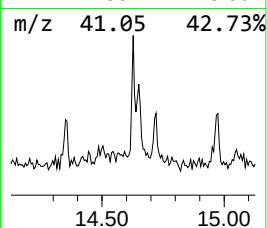
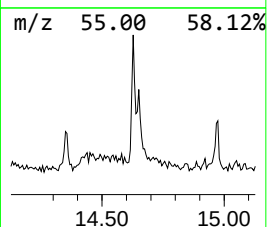
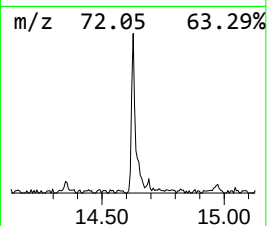
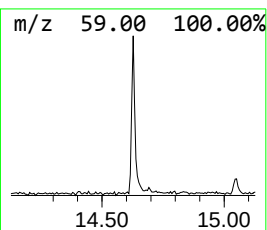
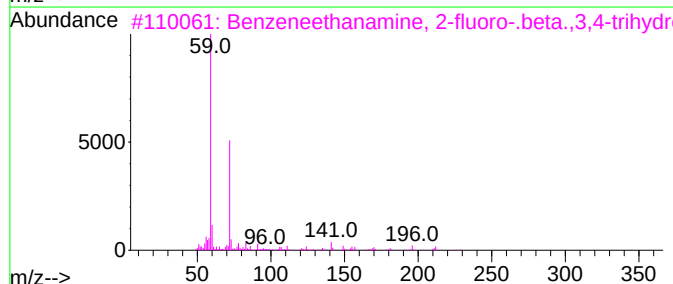
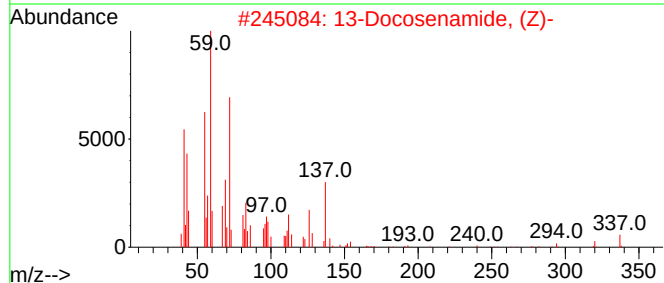
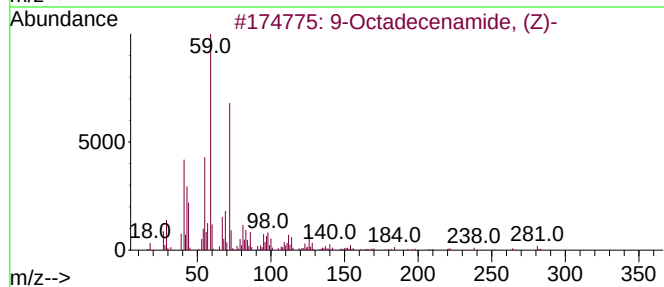
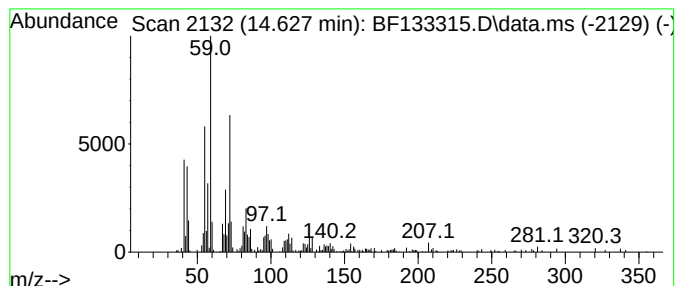
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.627	2.85 ng	162802	Perylene-d12	15.286

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	58
4		Palmitoleamide	253	C16H31NO	106010-22-4	58
5		Dodecanamide	199	C12H25NO	001120-16-7	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050923\
Data File : BF133315.D
Acq On : 09 May 2023 14:00
Operator : CG\JU
Sample : 02665-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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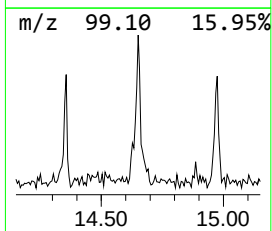
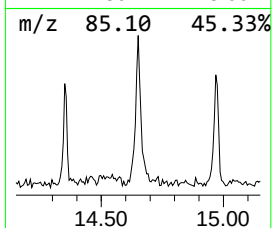
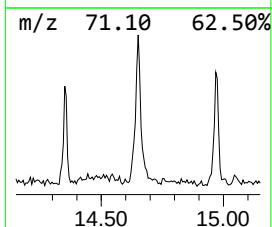
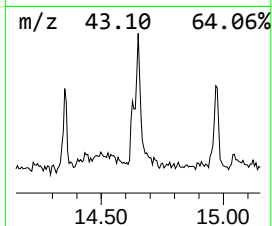
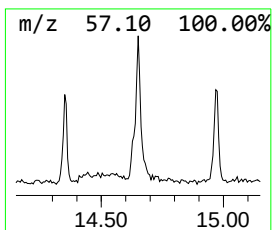
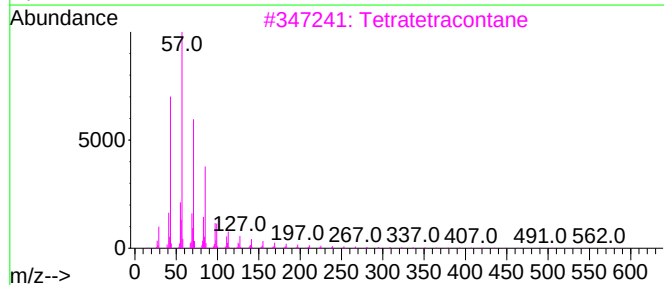
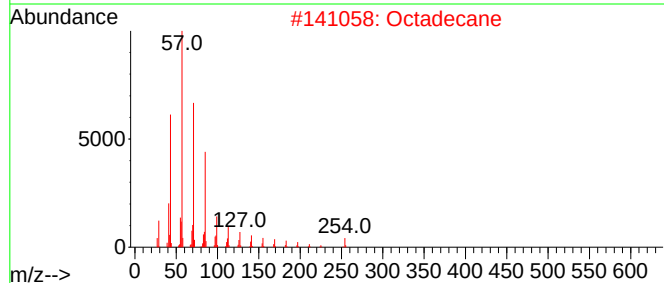
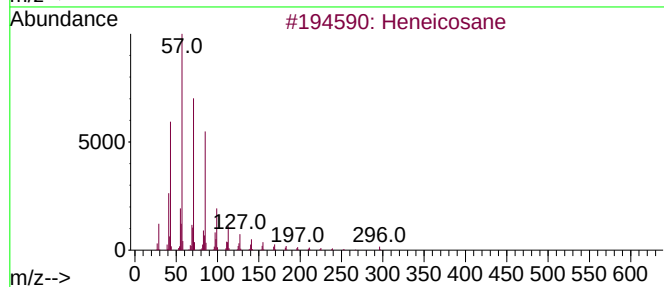
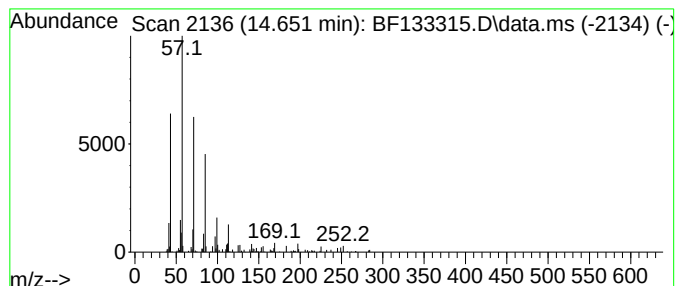
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.651	3.00 ng	171016	Perylene-d12	15.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	86
2			Octadecane	254	C18H38	000593-45-3	86
3			Tetratetracontane	619	C44H90	007098-22-8	78
4			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	78
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050923\
Data File : BF133315.D
Acq On : 09 May 2023 14:00
Operator : CG\JU
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ClientSampleId :
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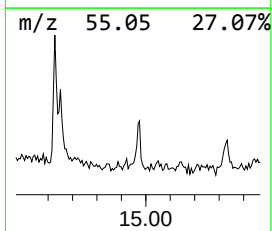
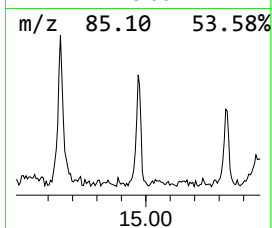
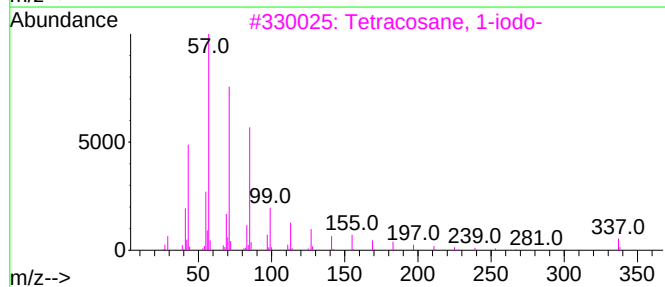
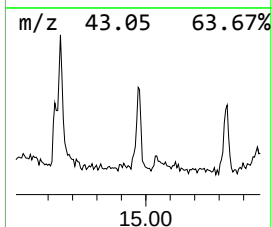
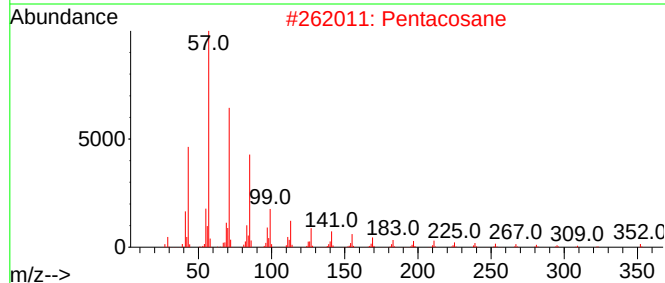
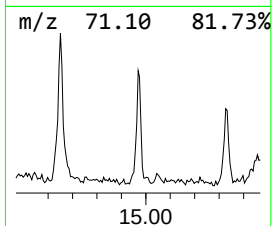
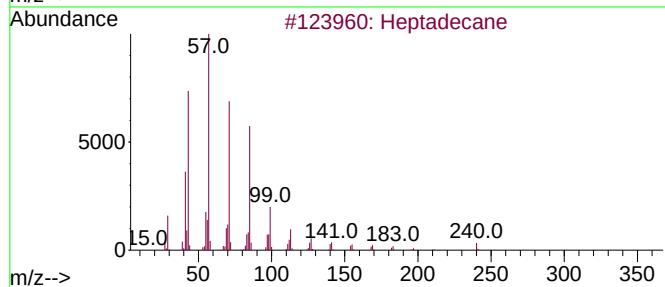
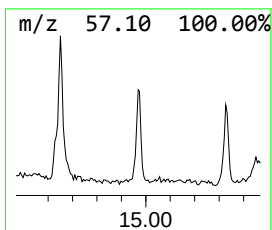
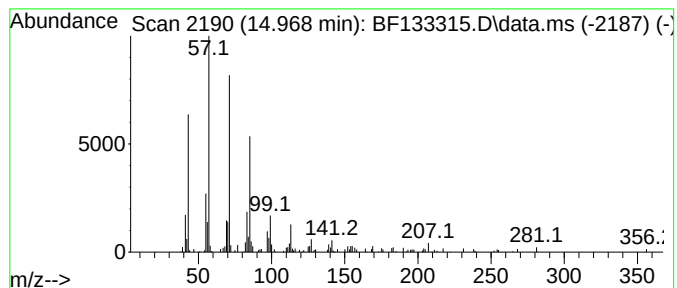
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	2.40 ng	136761	Perylene-d12	15.286

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	91
2		Pentacosane	352	C25H52	000629-99-2	90
3		Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	90
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
5		Hexadecane	226	C16H34	000544-76-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050923\
Data File : BF133315.D
Acq On : 09 May 2023 14:00
Operator : CG\JU
Sample : 02665-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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					#	RT	Resp	Conc
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Benzophenone	10.469	13.3	ng	1300650	3	9.757	1950190	20.0
Methanone, (1-h...	10.775	2.5	ng	251086	4	11.239	2026030	20.0
2-{2-[2-(Acrylo...	10.863	2.4	ng	241322	4	11.239	2026030	20.0
n-Hexadecanoic ...	11.775	7.1	ng	721539	4	11.239	2026030	20.0
Octadecanoic acid	12.557	11.8	ng	976896	5	13.868	1655340	20.0
n-Nonadecanol-1	13.763	7.0	ng	582849	5	13.868	1655340	20.0
9-Octadecenamid...	14.627	2.9	ng	162802	6	15.286	1140540	20.0
Heneicosane	14.651	3.0	ng	171016	6	15.286	1140540	20.0
Heptadecane	14.968	2.4	ng	136761	6	15.286	1140540	20.0