

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
 Data File : BF133275.D
 Acq On : 05 May 2023 21:20
 Operator : CG\JU
 Sample : 02624-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WZ-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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133275.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.922	477	482	495	rVB	603487	813593	18.87%	2.247%
2	5.346	549	554	557	rBV	3873096	4079374	94.63%	11.268%
3	6.369	723	728	731	rBV	4058525	4037331	93.65%	11.152%
4	6.722	785	788	792	rBV	1223808	1051097	24.38%	2.903%
5	7.292	880	885	888	rBV	2965041	2627623	60.95%	7.258%
6	8.010	1003	1007	1010	rBV	1779745	1392215	32.29%	3.845%
7	9.086	1186	1190	1193	rBV	5280344	4275782	99.18%	11.810%
8	9.757	1301	1304	1308	rBV	1942670	1559010	36.16%	4.306%
9	10.475	1422	1426	1429	rBV	916146	776725	18.02%	2.145%
10	10.551	1434	1439	1442	rBV	2817617	2760176	64.03%	7.624%
11	10.775	1474	1477	1480	rBV	89428	79184	1.84%	0.219%
12	11.239	1552	1556	1558	rBV	1957245	1604593	37.22%	4.432%
13	11.263	1558	1560	1563	rVV	375890	272328	6.32%	0.752%
14	11.310	1563	1568	1572	rVB	60631	65600	1.52%	0.181%
15	11.780	1644	1648	1652	rBV2	443135	459335	10.65%	1.269%
16	11.851	1657	1660	1662	rBV	57372	54016	1.25%	0.149%
17	12.445	1758	1761	1765	rBV	445659	425578	9.87%	1.176%
18	12.563	1777	1781	1786	rBV2	101673	132665	3.08%	0.366%
19	12.674	1794	1800	1803	rBV	392790	374524	8.69%	1.034%
20	12.827	1822	1826	1829	rBV	4591201	4311046	100.00%	11.908%
21	13.069	1860	1867	1870	rBV2	69216	88230	2.05%	0.244%
22	13.410	1922	1925	1927	rBV	64432	60491	1.40%	0.167%
23	13.727	1974	1979	1996	rBV3	281172	514403	11.93%	1.421%
24	13.874	1998	2004	2006	rBV	1332338	1364266	31.65%	3.768%
25	13.898	2006	2008	2011	rVV	141390	112178	2.60%	0.310%
26	13.969	2014	2020	2026	rBV	960067	989238	22.95%	2.732%
27	14.051	2031	2034	2038	rVB2	77789	73482	1.70%	0.203%
28	14.357	2082	2086	2089	rBV	94739	106903	2.48%	0.295%
29	14.651	2133	2136	2143	rVB	69728	67563	1.57%	0.187%
30	14.721	2145	2148	2155	rVB3	36332	54934	1.27%	0.152%
31	14.886	2172	2176	2179	rBV	102150	157618	3.66%	0.435%
32	14.974	2187	2191	2198	rBV3	68235	93508	2.17%	0.258%
33	15.168	2221	2224	2229	rVB	65746	77516	1.80%	0.214%
34	15.227	2230	2234	2238	rBV	81271	97880	2.27%	0.270%
35	15.286	2240	2244	2249	rBV	816155	977972	22.69%	2.701%
36	15.739	2317	2321	2326	rBV	46735	64592	1.50%	0.178%

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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	16.657	2472	2477	2485	rVB4	40248	86732	2.01%	0.240%
38	17.062	2543	2546	2558	rVB3	33084	64689	1.50%	0.179%

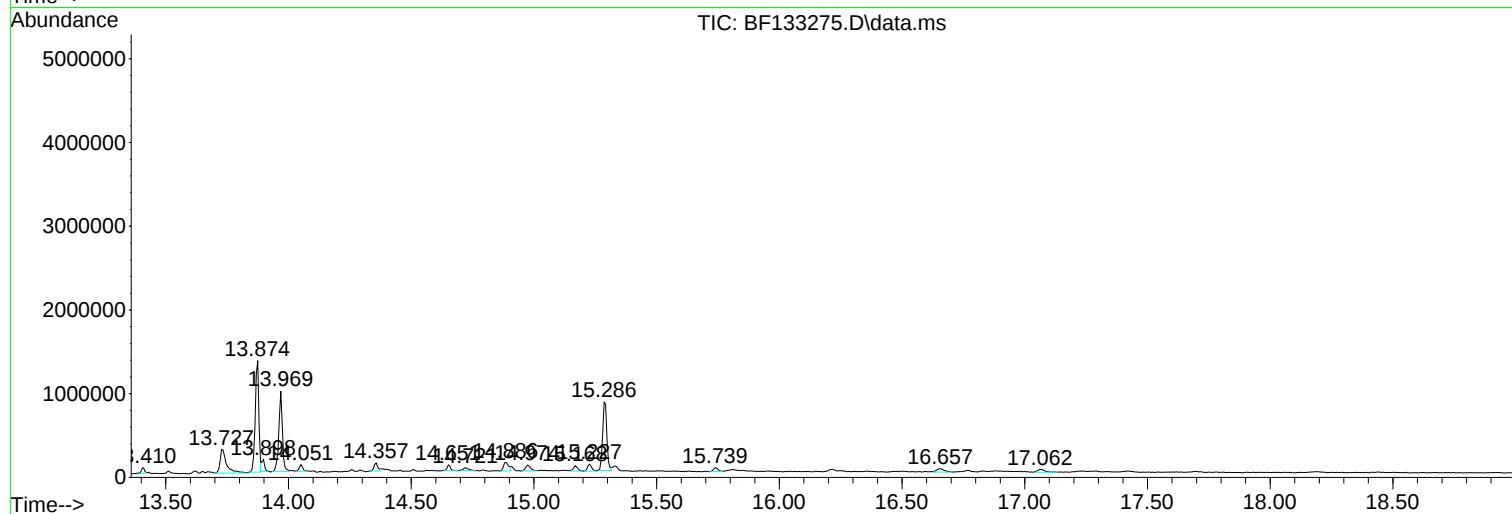
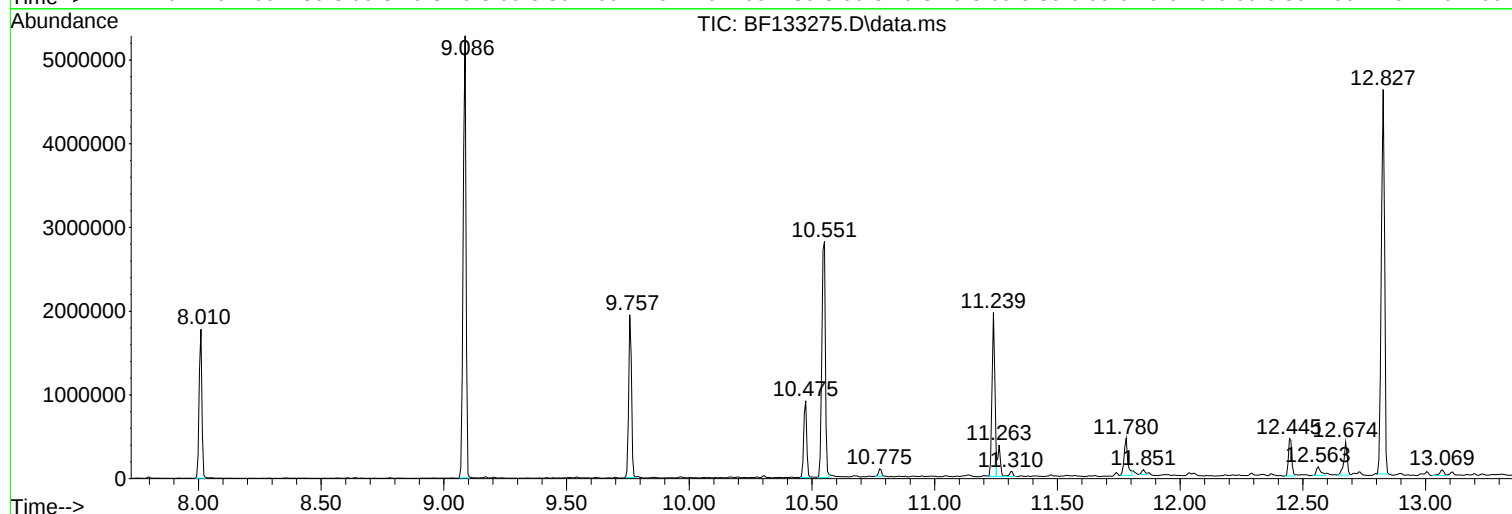
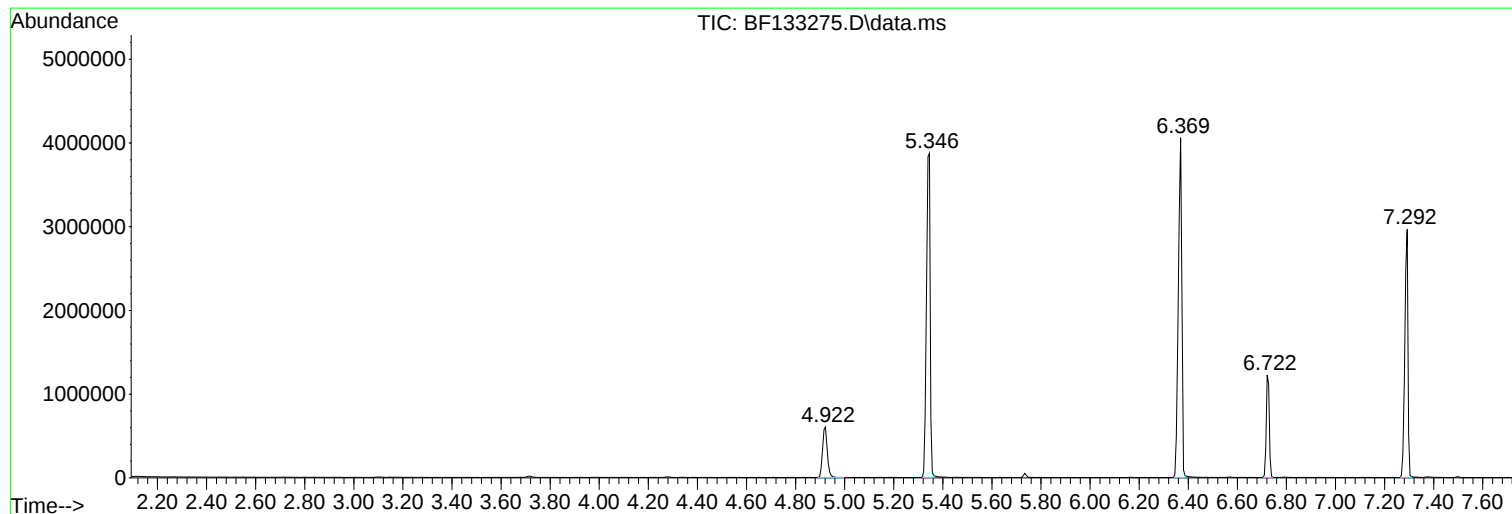
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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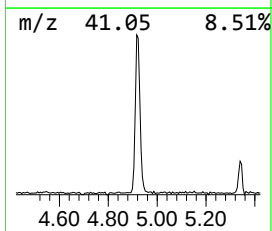
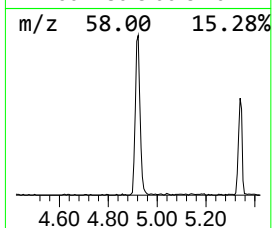
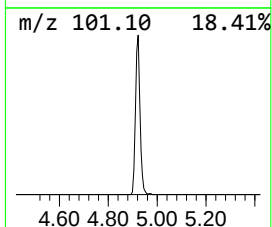
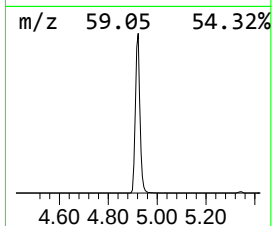
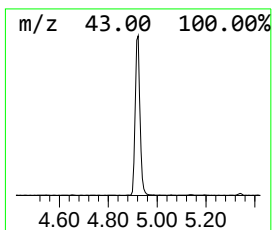
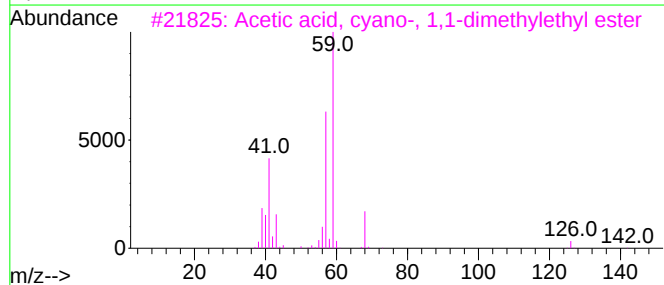
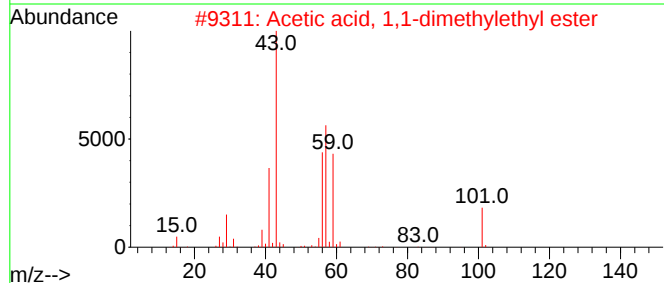
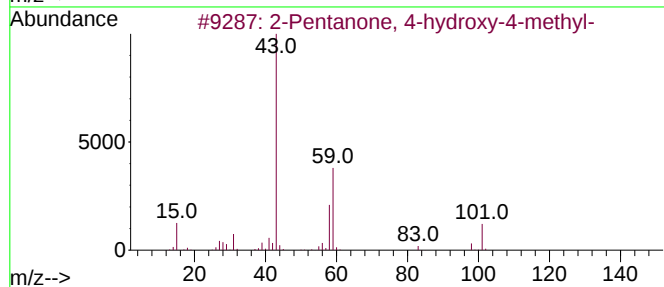
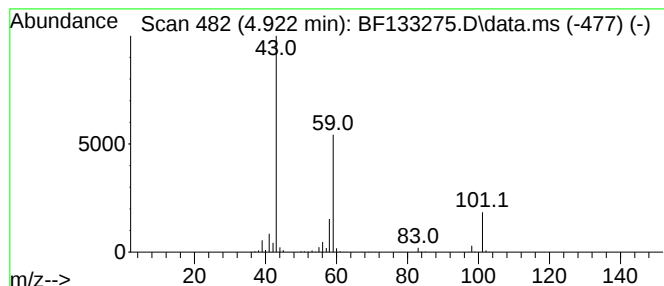
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.922	15.48 ng	813593	1,4-Dichlorobenzene-d4	6.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9		



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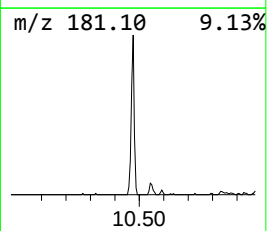
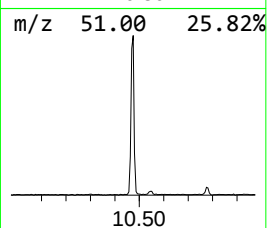
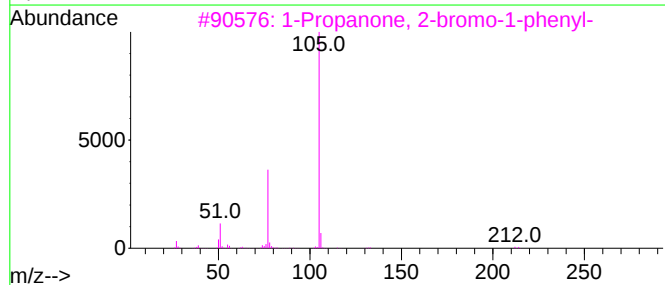
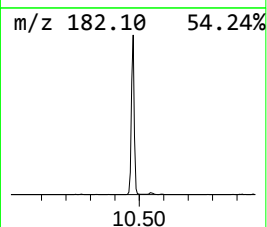
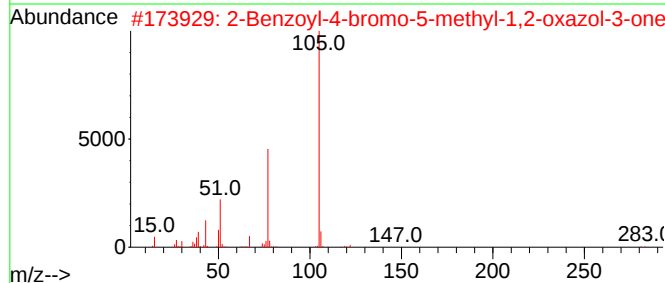
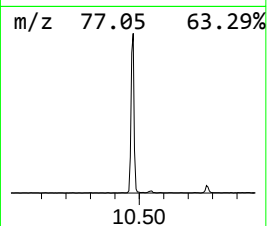
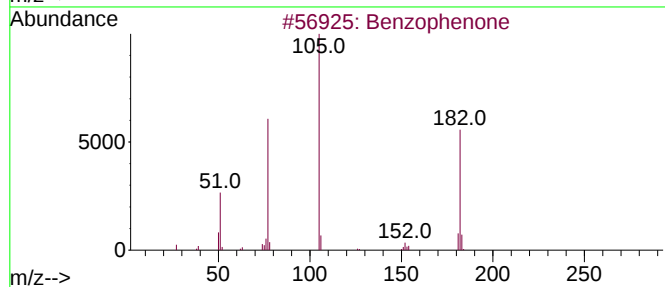
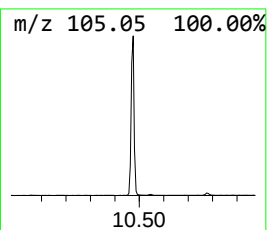
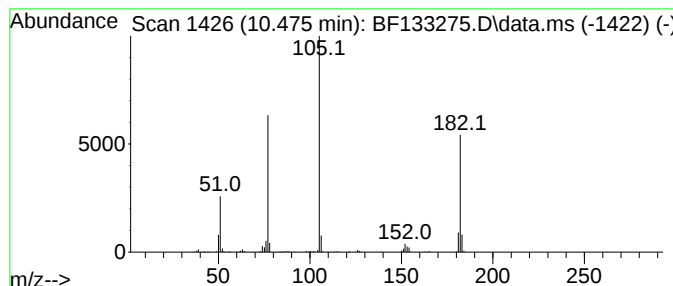
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	9.96 ng	776725	Acenaphthene-d10	9.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4			Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47



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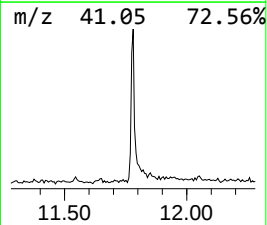
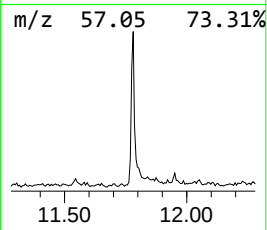
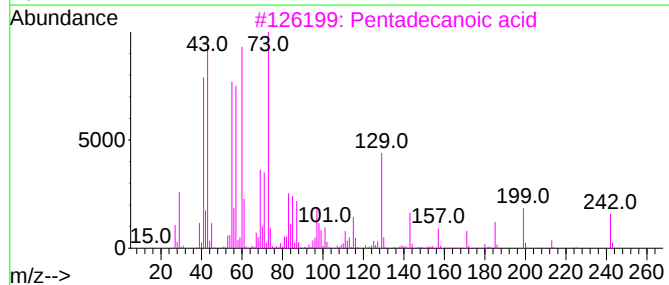
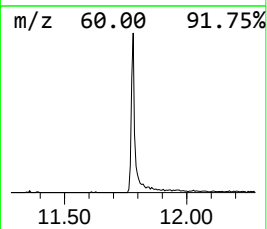
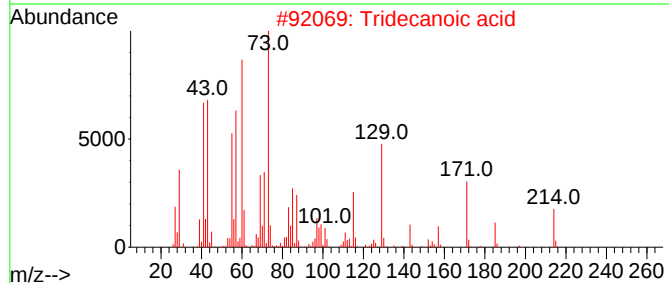
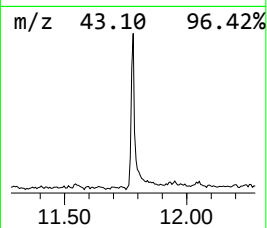
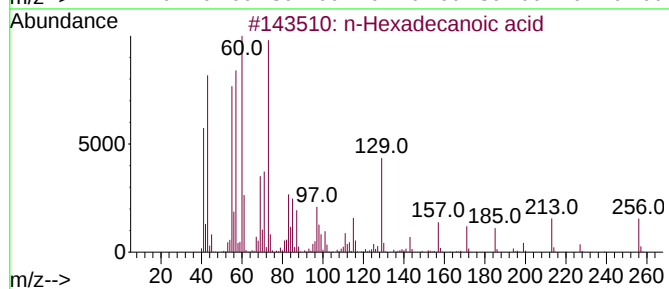
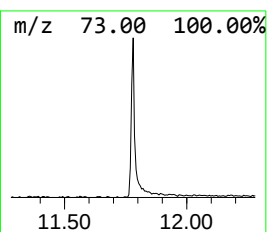
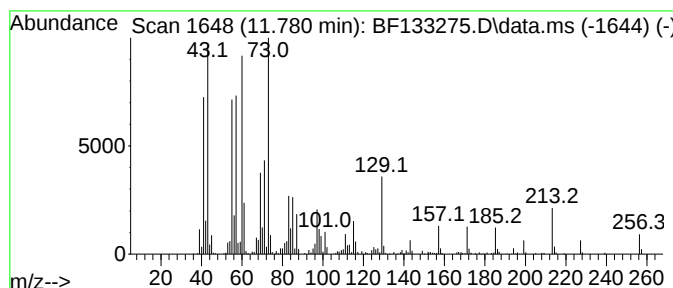
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.780	5.73 ng	459335	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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Nonanoic acid	158	C9H18O2	000112-05-0	43



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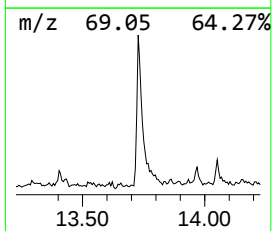
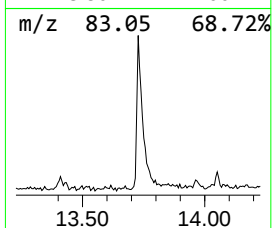
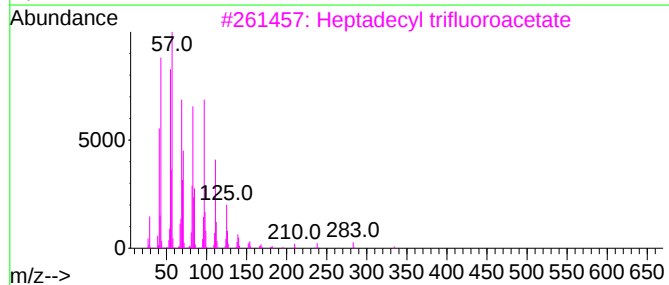
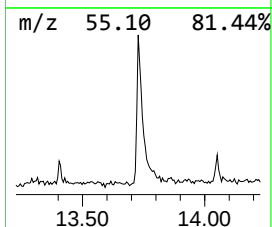
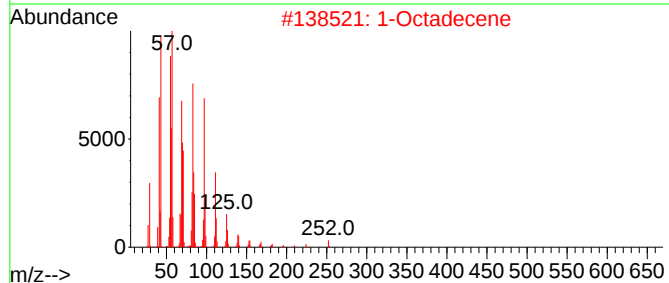
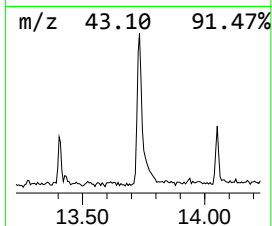
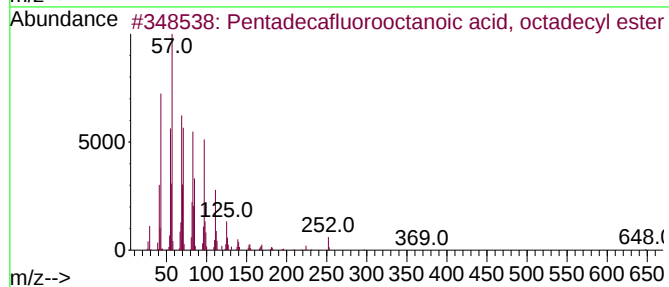
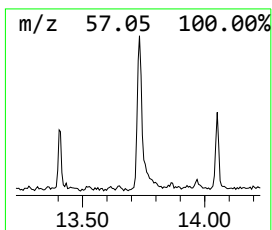
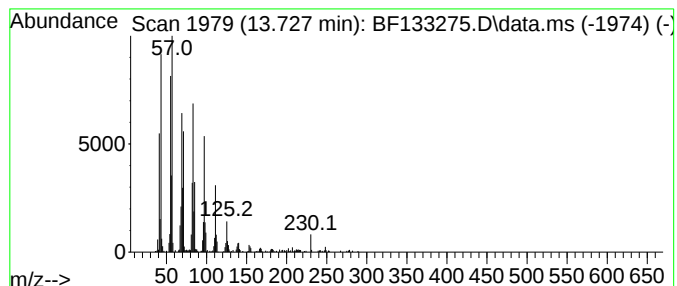
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Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	7.54 ng	514403	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			1-Octadecene	252	C18H36	000112-88-9	93
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	93
4			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
5			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	90



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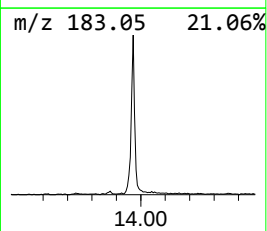
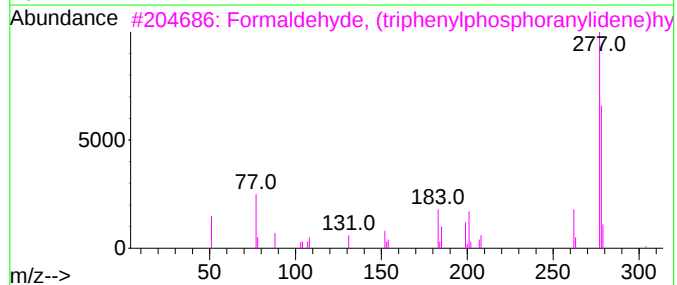
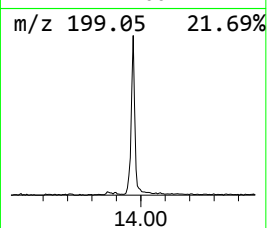
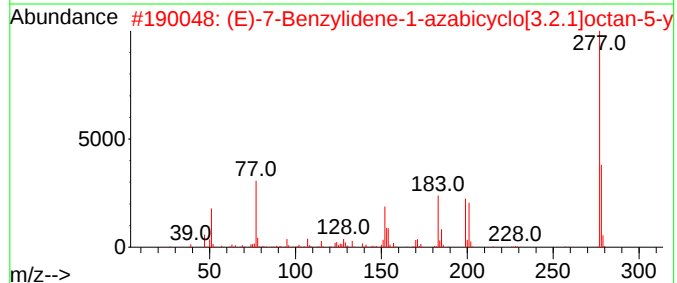
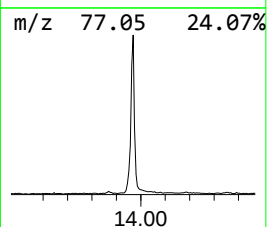
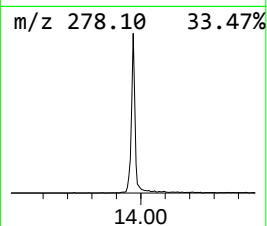
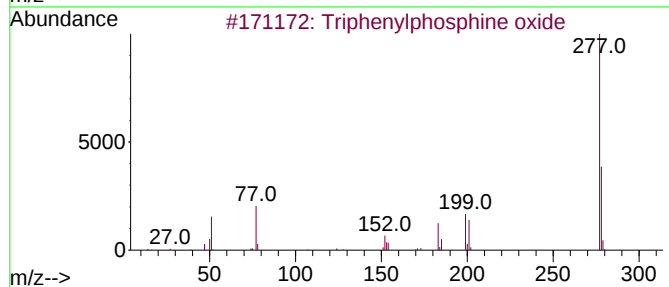
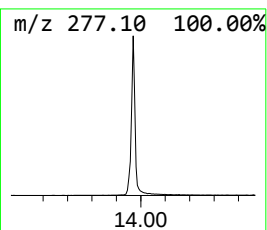
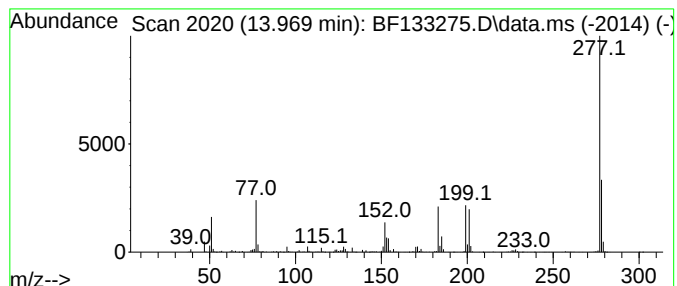
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.969	14.50 ng	989238	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	76
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	50
4			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	32
5			4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133275.D
Acq On : 05 May 2023 21:20
Operator : CG\JU
Sample : 02624-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WZ-3

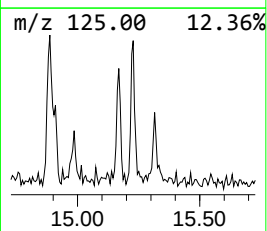
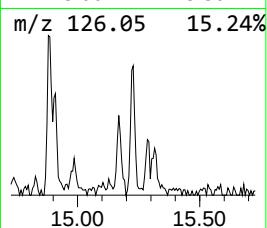
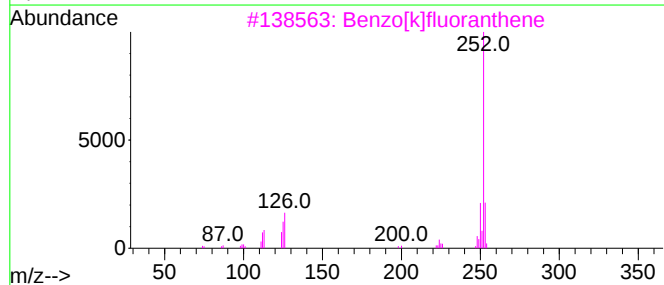
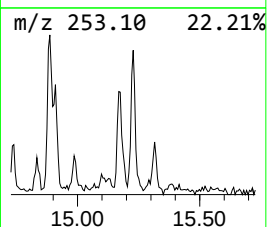
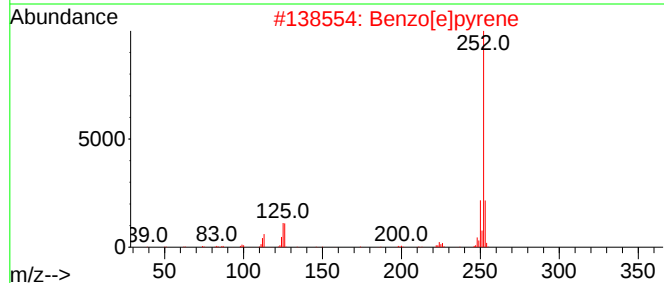
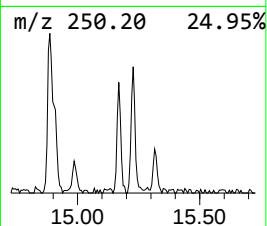
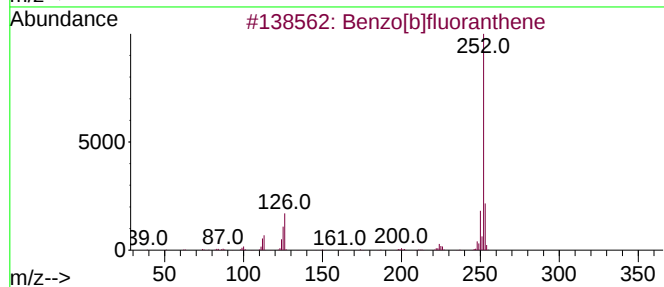
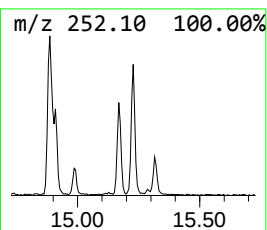
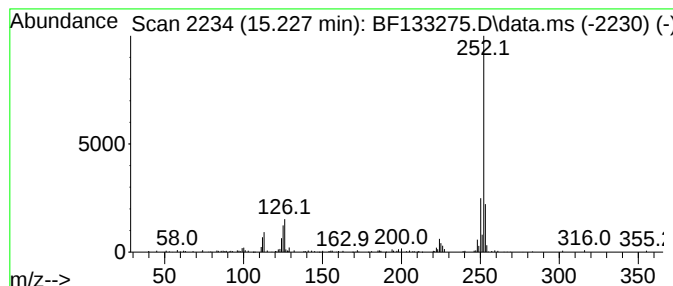
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.227	2.00 ng	97880	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
2			Benzo[e]pyrene	252	C20H12	000192-97-2	96
3			Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4			Benzo[a]pyrene	252	C20H12	000050-32-8	95
5			Perylene	252	C20H12	000198-55-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133275.D
Acq On : 05 May 2023 21:20
Operator : CG\JU
Sample : 02624-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WZ-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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-...	4.922	15.5	ng	813593	1	6.728	1051100	20.0
Benzophenone	10.475	10.0	ng	776725	3	9.757	1559010	20.0
n-Hexadecanoic ...	11.780	5.7	ng	459335	4	11.239	1604590	20.0
Pentadecafluoro...	13.727	7.5	ng	514403	5	13.874	1364270	20.0
Triphenylphosph...	13.969	14.5	ng	989238	5	13.874	1364270	20.0
Benzo[e]pyrene	15.227	2.0	ng	97880	6	15.292	977972	20.0