

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
 Data File : BF133160.D
 Acq On : 01 May 2023 17:34
 Operator : CG\JU
 Sample : 02495-05
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GMW-11

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: BF133160.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.910	477	480	488	rVB	55140	66244	1.17%	0.185%
2	5.304	543	547	549	rBV2	96600	104776	1.85%	0.293%
3	5.340	549	553	556	rVB	2355149	2305161	40.77%	6.446%
4	6.363	723	727	730	rBV	1785489	1427439	25.25%	3.991%
5	6.728	785	789	792	rBV	1472923	1111420	19.66%	3.108%
6	7.292	879	885	888	rBV	3384056	3467266	61.32%	9.695%
7	7.757	956	964	967	rBV2	192713	166216	2.94%	0.465%
8	8.010	1004	1007	1009	rBV	1753181	1546335	27.35%	4.324%
9	8.033	1009	1011	1014	rVB	1294588	924583	16.35%	2.585%
10	8.722	1123	1128	1132	rBV	149887	130940	2.32%	0.366%
11	8.822	1141	1145	1149	rBV	138776	108543	1.92%	0.304%
12	9.092	1185	1191	1194	rBV	6560538	5653951	100.00%	15.809%
13	9.763	1301	1305	1308	rBV	2171872	1744501	30.85%	4.878%
14	9.798	1308	1311	1314	rVB	226274	194843	3.45%	0.545%
15	9.969	1336	1340	1344	rBV	144240	139002	2.46%	0.389%
16	10.051	1348	1354	1358	rBV	36790	64244	1.14%	0.180%
17	10.310	1395	1398	1401	rBV	166677	136966	2.42%	0.383%
18	10.480	1423	1427	1430	rBV	978584	772790	13.67%	2.161%
19	10.557	1435	1440	1443	rBV	3559826	3553488	62.85%	9.936%
20	10.786	1476	1479	1485	rVB2	66413	74486	1.32%	0.208%
21	11.245	1554	1557	1560	rBV	2184731	1798941	31.82%	5.030%
22	11.269	1560	1561	1564	rVB	216468	108026	1.91%	0.302%
23	11.474	1593	1596	1600	rVB	272973	210036	3.71%	0.587%
24	11.786	1644	1649	1658	rBV2	686669	711577	12.59%	1.990%
25	12.568	1779	1782	1793	rVB	494824	492950	8.72%	1.378%
26	12.721	1805	1808	1813	rVB2	62680	68089	1.20%	0.190%
27	12.839	1823	1828	1831	rBV	5428004	5380069	95.16%	15.043%
28	13.074	1865	1868	1872	rBV	66599	69070	1.22%	0.193%
29	13.415	1923	1926	1930	rVB	95158	90974	1.61%	0.254%
30	13.680	1969	1971	1978	rVB	97855	97700	1.73%	0.273%
31	13.745	1979	1982	1984	rBV	110753	121922	2.16%	0.341%
32	13.768	1984	1986	1996	rVB2	144928	283688	5.02%	0.793%
33	13.880	2001	2005	2008	rBV	1233446	1076262	19.04%	3.009%
34	14.062	2033	2036	2042	rVB	107821	101617	1.80%	0.284%
35	14.368	2085	2088	2091	rVB	103252	92488	1.64%	0.259%
36	14.662	2136	2138	2143	rVB	75000	75725	1.34%	0.212%

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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	14.733	2147	2150	2159	rVB	92520	117040	2.07%	0.327%
38	14.986	2190	2193	2199	rVB	77578	86848	1.54%	0.243%
39	15.298	2241	2246	2251	rBV	898162	1019573	18.03%	2.851%
40	15.762	2321	2325	2330	rVB2	49645	67850	1.20%	0.190%

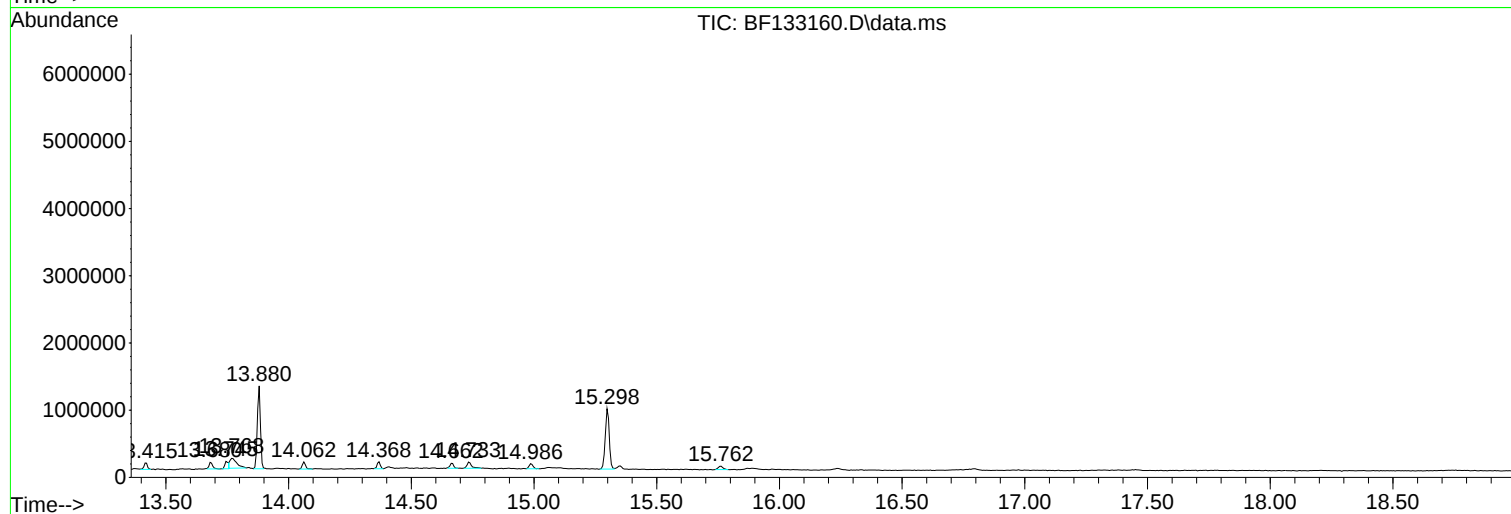
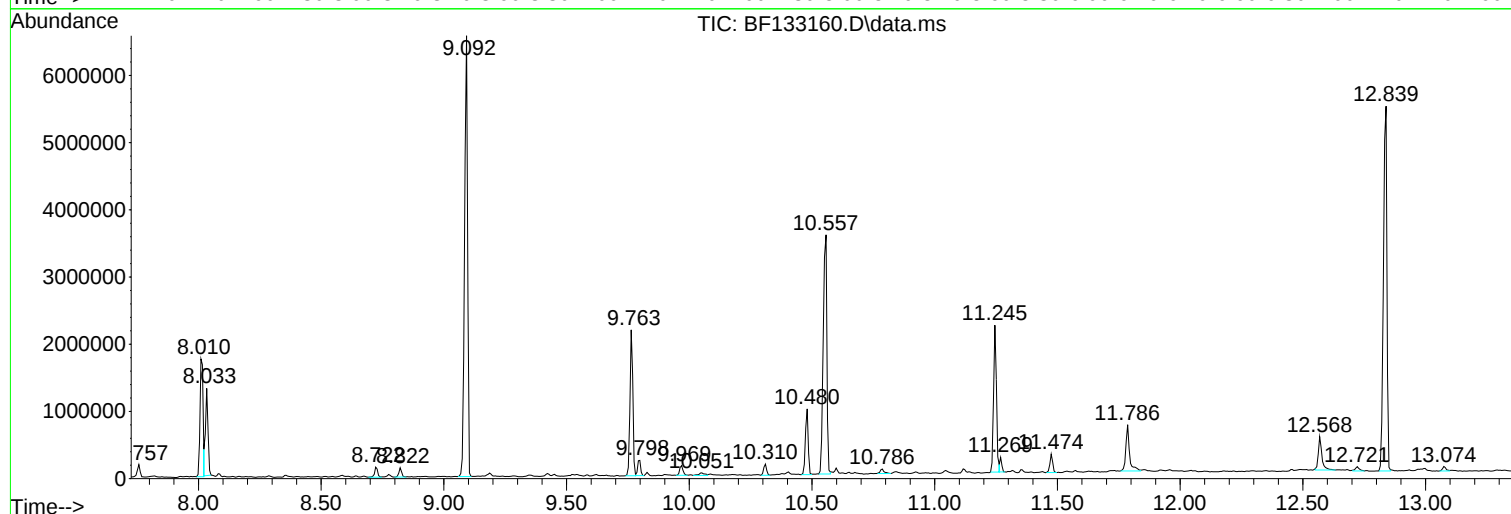
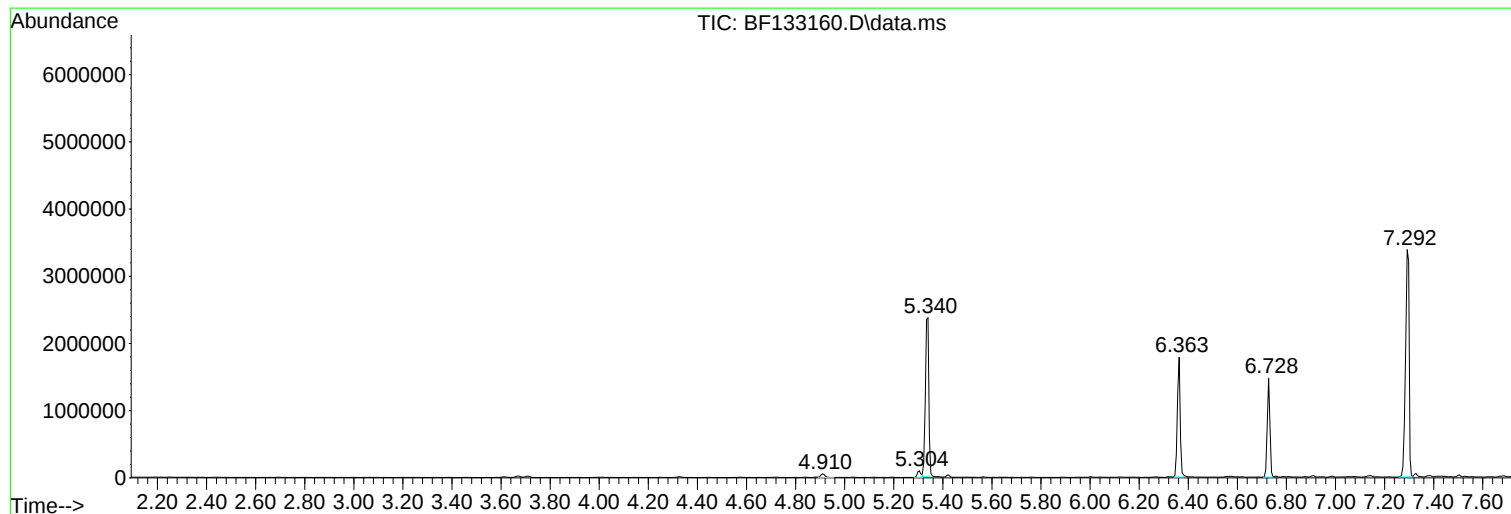
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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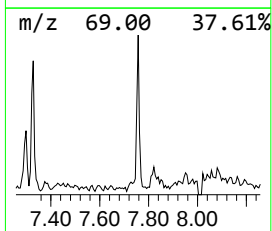
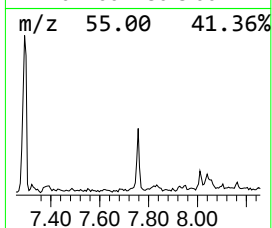
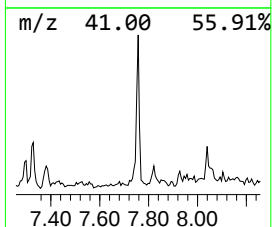
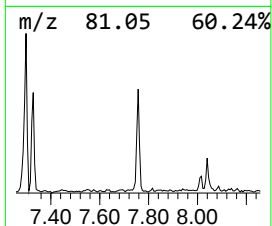
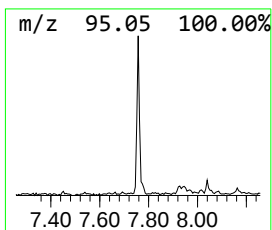
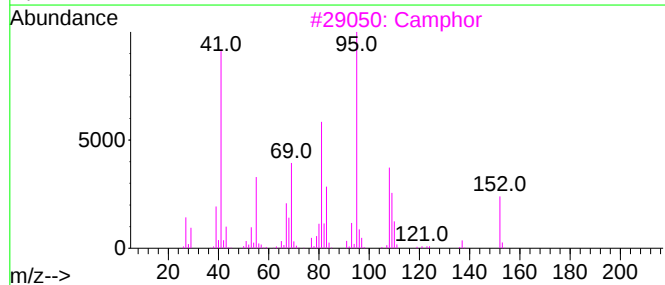
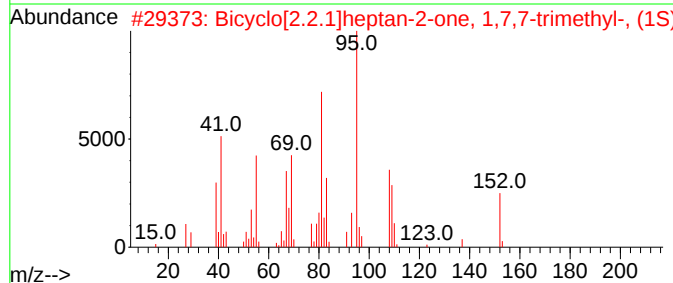
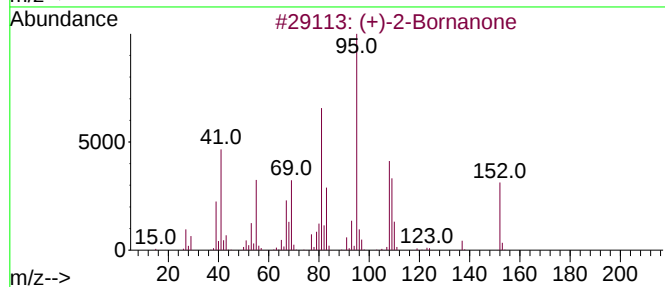
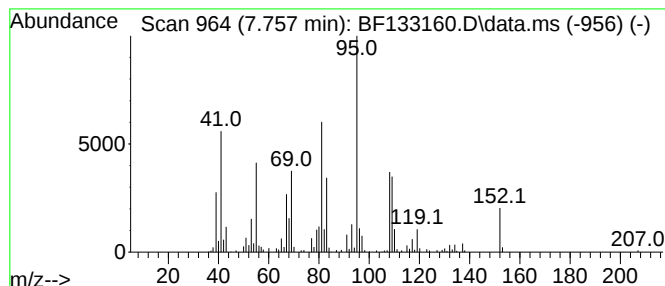
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (+)-2-Bornanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
7.757	2.15 ng	166216	Naphthalene-d8	8.010	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	97
2	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	97
3	Camphor	152	C10H16O	000076-22-2	96
4	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	46
5	1-Adamantanol	152	C10H16O	000768-95-6	43



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Misc :
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Instrument :
BNA_F
ClientSampleId :
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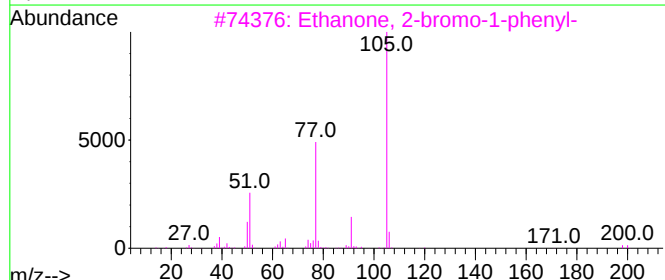
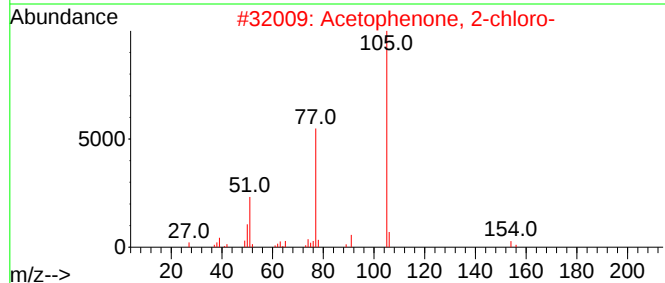
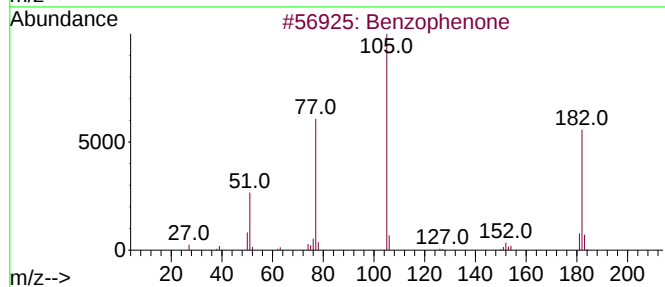
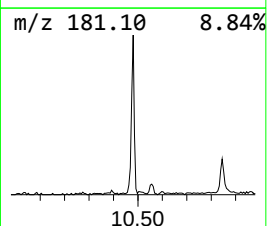
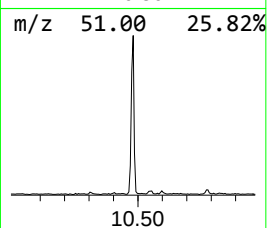
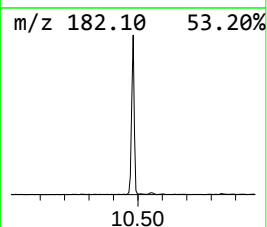
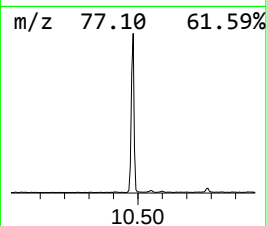
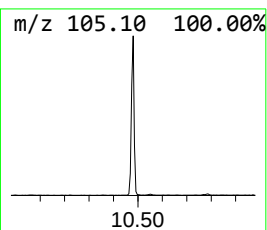
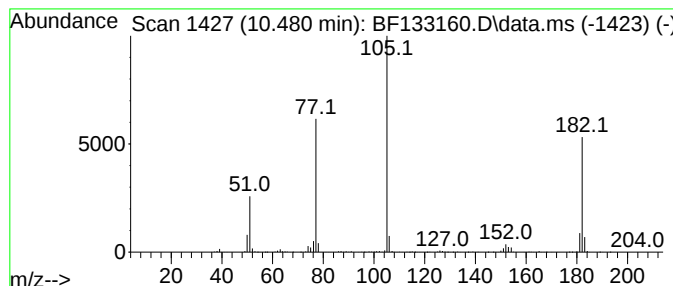
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.480	8.86 ng	772790	Acenaphthene-d10	9.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			Ethanone, 2-bromo-1-phenyl-	198	C8H7BrO	000070-11-1	47
4			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
5			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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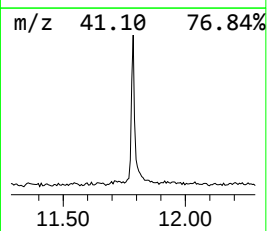
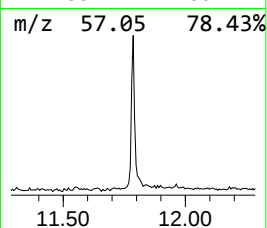
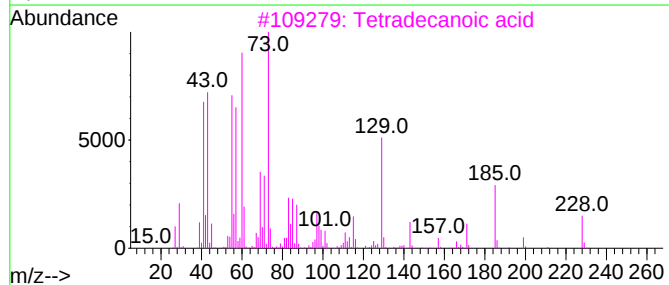
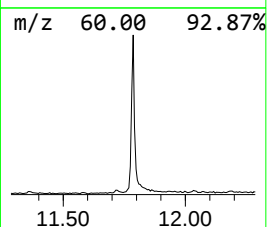
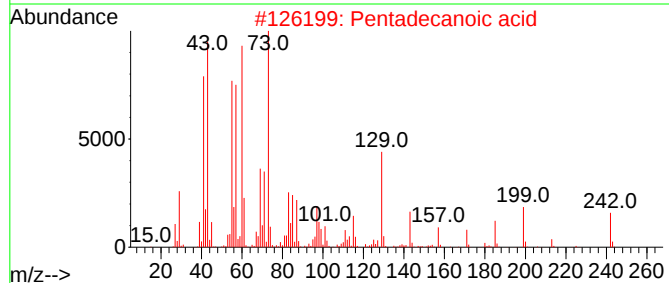
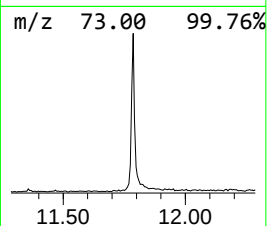
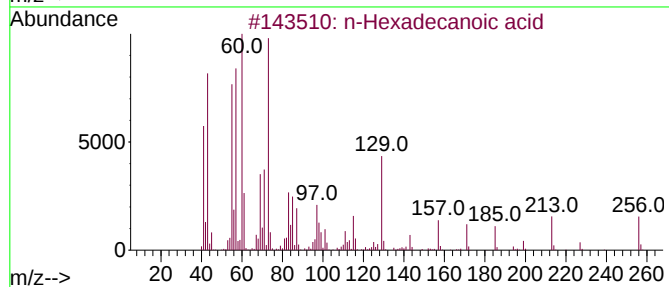
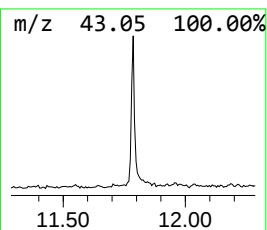
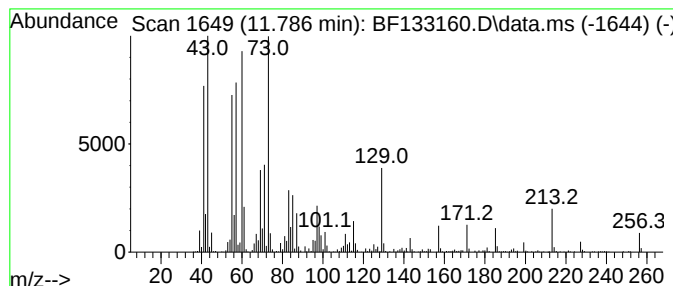
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	7.91 ng	711577	Phenanthrene-d10	11.245

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	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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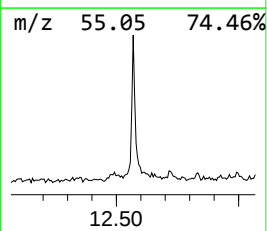
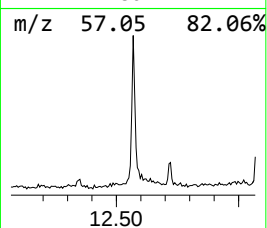
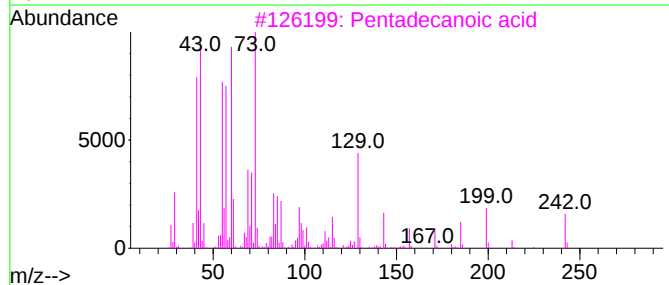
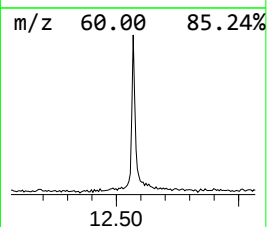
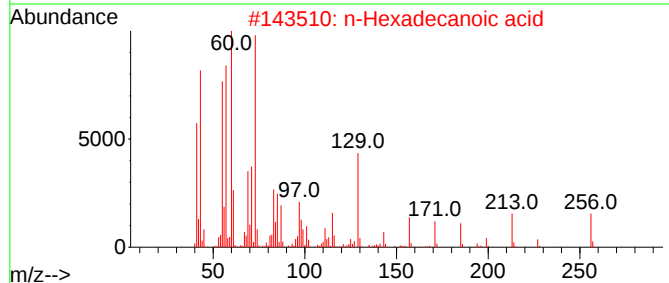
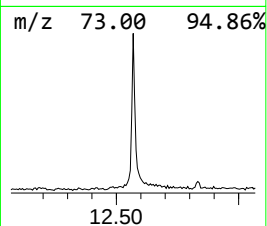
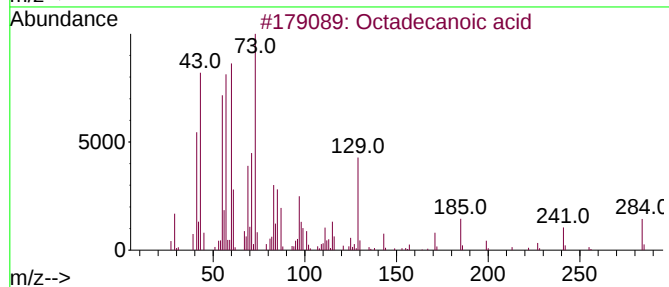
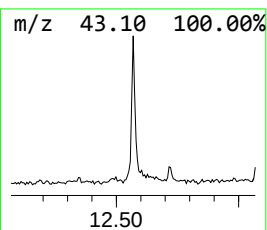
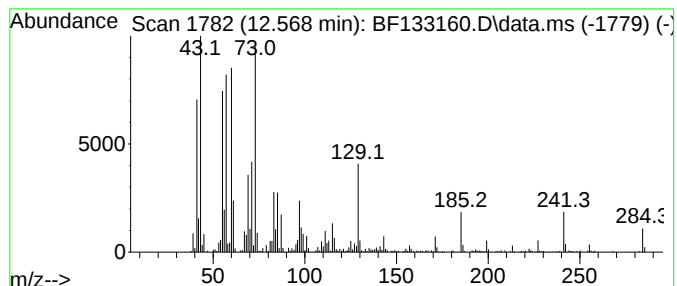
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.569	9.16 ng	492950	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



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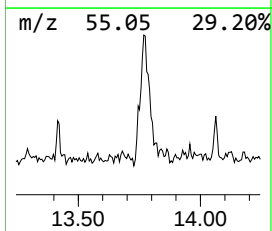
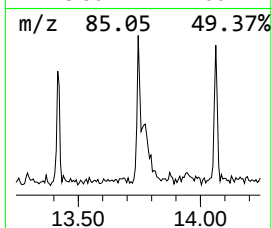
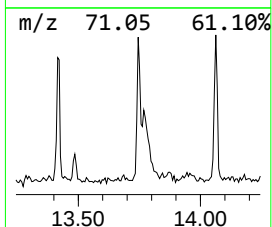
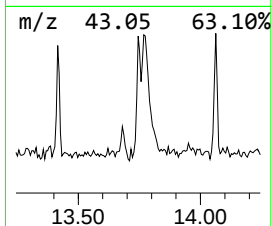
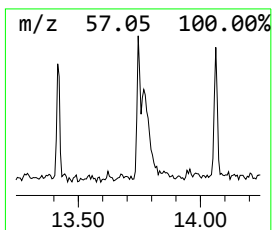
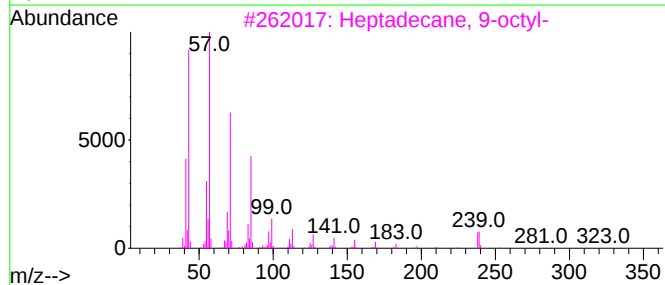
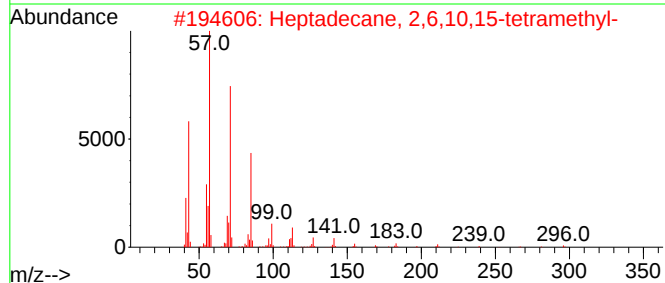
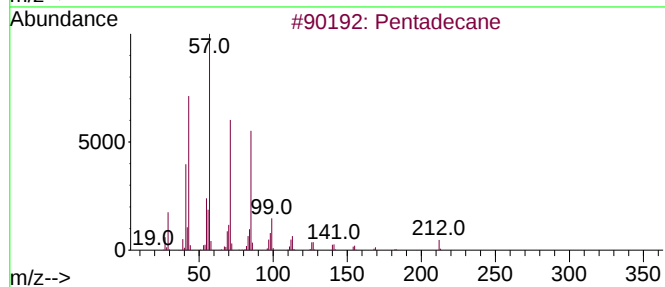
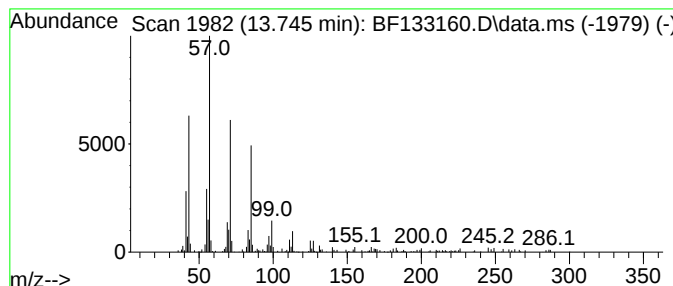
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.745	2.27 ng	121922	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	87
2			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
4			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
5			Heptadecane	240	C17H36	000629-78-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133160.D
Acq On : 01 May 2023 17:34
Operator : CG\JU
Sample : 02495-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GMW-11

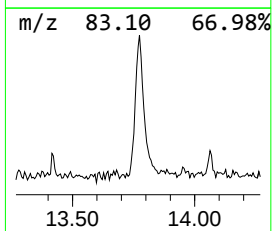
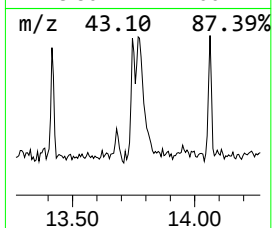
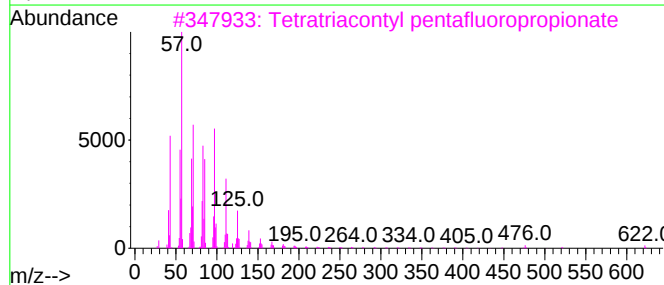
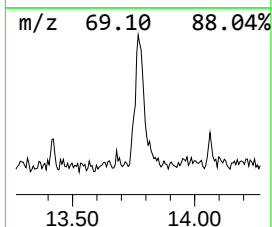
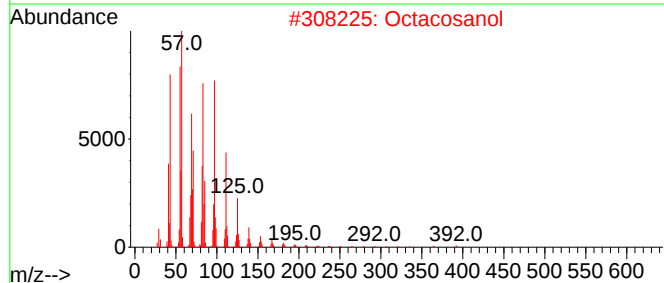
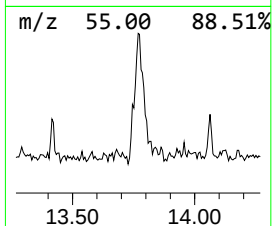
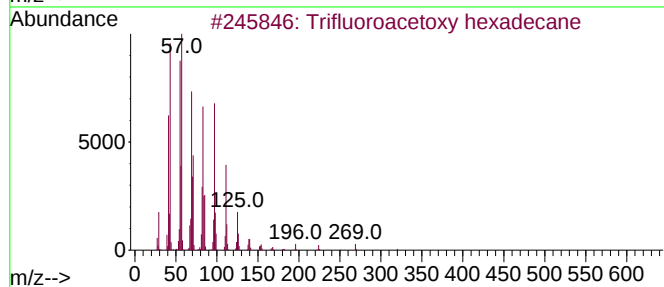
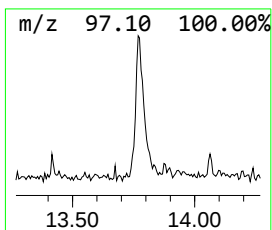
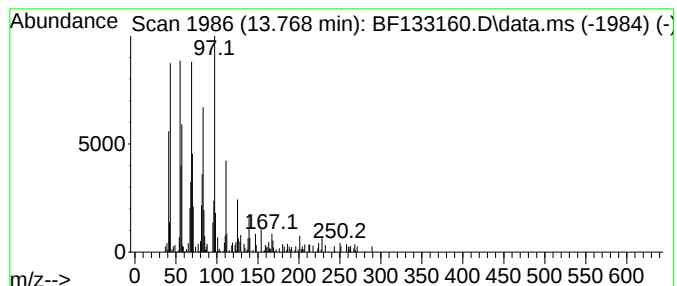
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.768	5.27 ng	283688	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	72
2			Octacosanol	410	C28H58O	000557-61-9	62
3			Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	58
4			Hexatriacontyl trifluoroacetate	619	C38H73F3O2	1000351-88-6	58
5			Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133160.D
Acq On : 01 May 2023 17:34
Operator : CG\JU
Sample : 02495-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GMW-11

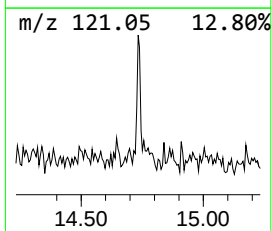
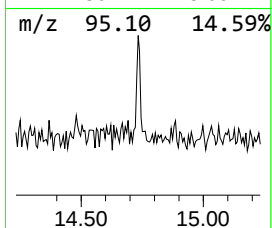
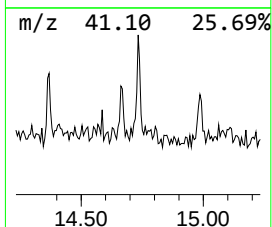
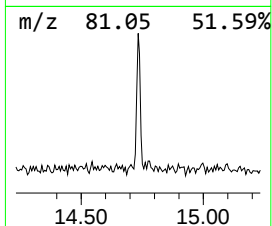
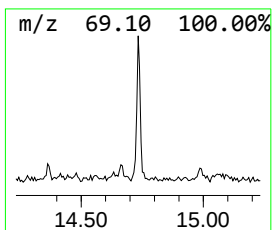
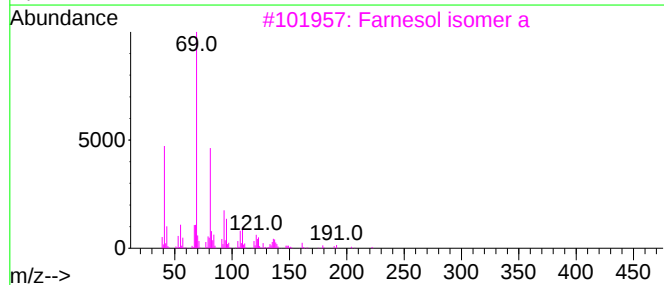
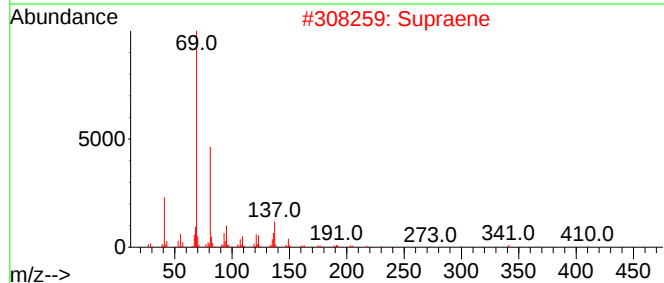
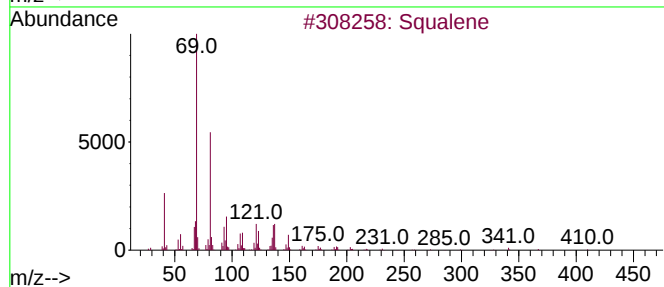
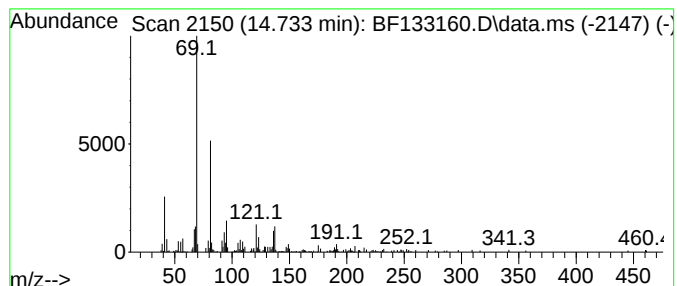
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	2.30 ng	117040	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	86
2			Supraene	410	C30H50	007683-64-9	83
3			Farnesol isomer a	222	C15H26O	1000108-92-4	81
4			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050123\
Data File : BF133160.D
Acq On : 01 May 2023 17:34
Operator : CG\JU
Sample : 02495-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GMW-11

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-Bornanone	7.757	2.1	ng	166216	2	8.010	1546340	20.0
Benzophenone	10.480	8.9	ng	772790	3	9.763	1744500	20.0
n-Hexadecanoic ...	11.786	7.9	ng	711577	4	11.245	1798940	20.0
Octadecanoic acid	12.569	9.2	ng	492950	5	13.880	1076260	20.0
Pentadecane	13.745	2.3	ng	121922	5	13.880	1076260	20.0
Trifluoroacetox...	13.768	5.3	ng	283688	5	13.880	1076260	20.0
Squalene	14.733	2.3	ng	117040	6	15.298	1019570	20.0