

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
 Data File : BF142369.D
 Acq On : 14 May 2025 16:46
 Operator : RC/JU
 Sample : Q2004-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 2811

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-BF050525.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142369.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.110	485	496	504	rBV	302876	469738	7.27%	1.227%
2	5.510	557	564	569	rBV	2756146	3877863	60.03%	10.128%
3	6.516	729	735	741	rVB	2844986	4120093	63.78%	10.760%
4	6.898	795	800	805	rBV	799486	963791	14.92%	2.517%
5	7.457	888	895	901	rBV	1950806	2723501	42.16%	7.113%
6	7.710	934	938	944	rBV	61737	74723	1.16%	0.195%
7	8.181	1013	1018	1026	rVB	1064182	1323408	20.49%	3.456%
8	9.257	1195	1201	1206	rBV	4278390	5564193	86.14%	14.532%
9	9.939	1311	1317	1327	rVB	1233933	1633742	25.29%	4.267%
10	10.651	1432	1438	1444	rBV	282813	353792	5.48%	0.924%
11	10.728	1444	1451	1456	rBV	2864238	3831254	59.31%	10.006%
12	11.422	1564	1569	1576	rVB	1393846	1744449	27.01%	4.556%
13	11.633	1601	1605	1615	rBV	90325	131603	2.04%	0.344%
14	11.951	1653	1659	1672	rBV2	721252	1175056	18.19%	3.069%
15	12.733	1787	1792	1806	rBV	101449	195577	3.03%	0.511%
16	13.016	1833	1840	1845	rBV	4662529	6459629	100.00%	16.870%
17	13.904	1986	1991	2009	rBV	226048	445125	6.89%	1.163%
18	14.063	2010	2018	2026	rBV2	1135353	1902298	29.45%	4.968%
19	14.692	2121	2125	2131	rBV	53125	71505	1.11%	0.187%
20	15.551	2265	2271	2288	rVB	745225	1228392	19.02%	3.208%

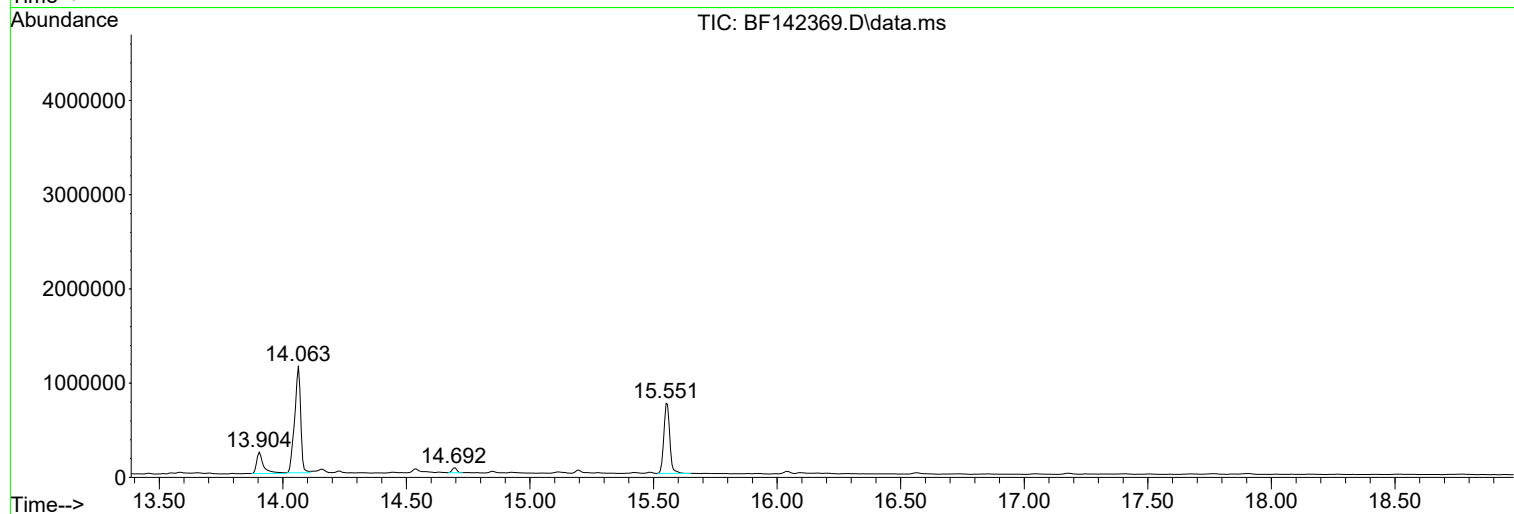
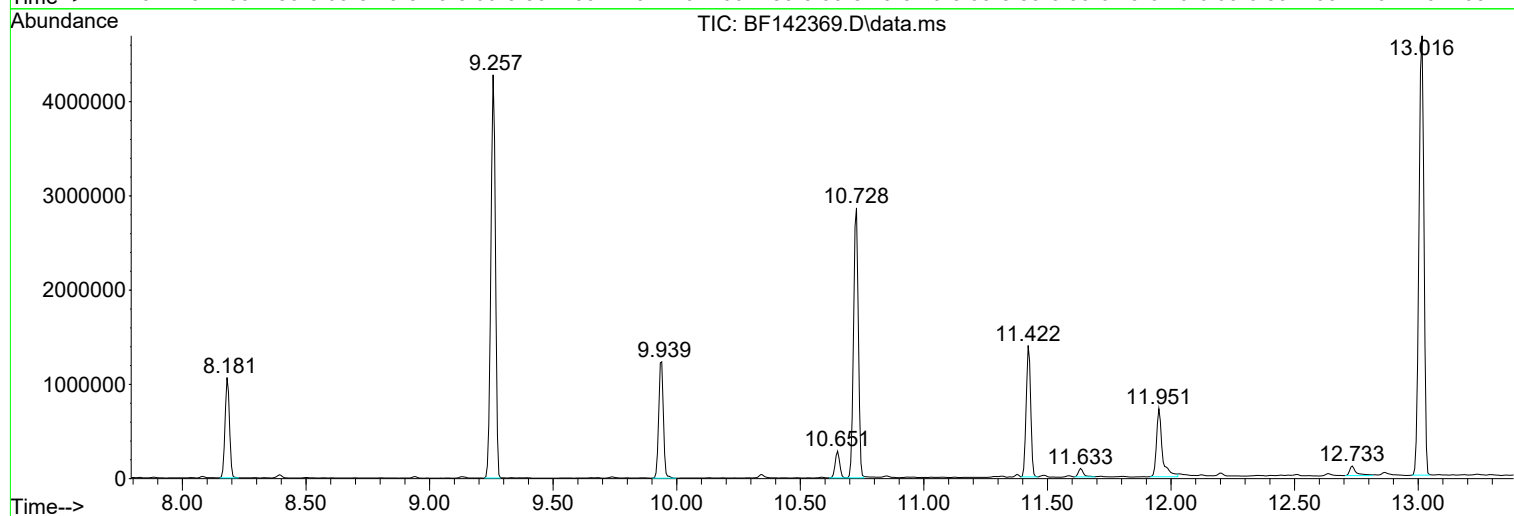
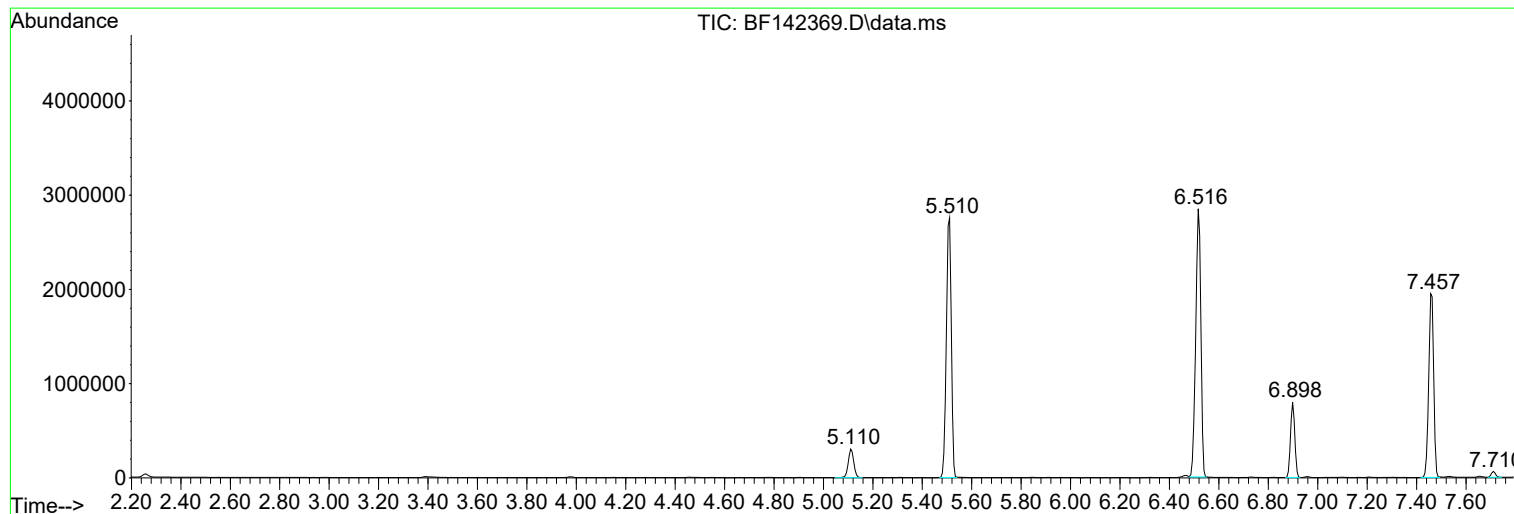
Sum of corrected areas: 38289732

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
Data File : BF142369.D
Acq On : 14 May 2025 16:46
Operator : RC/JU
Sample : Q2004-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2811

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
Data File : BF142369.D
Acq On : 14 May 2025 16:46
Operator : RC/JU
Sample : Q2004-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2811

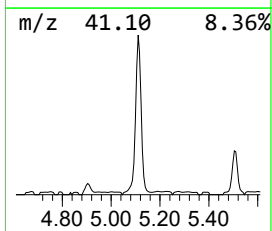
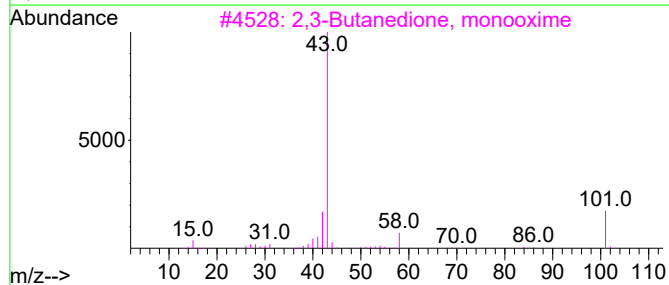
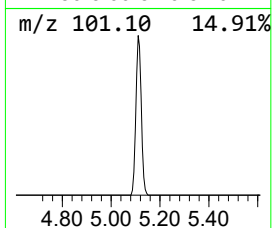
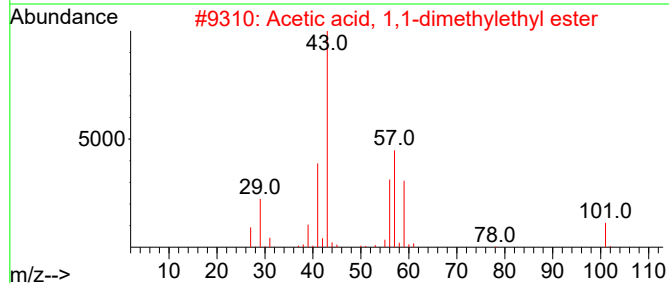
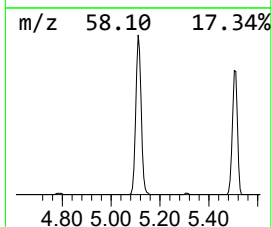
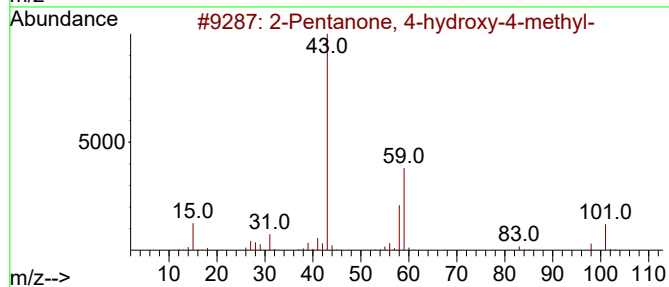
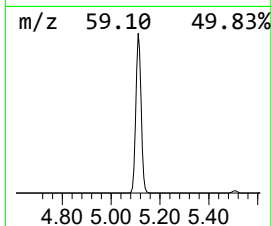
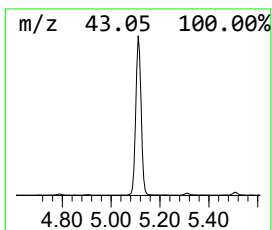
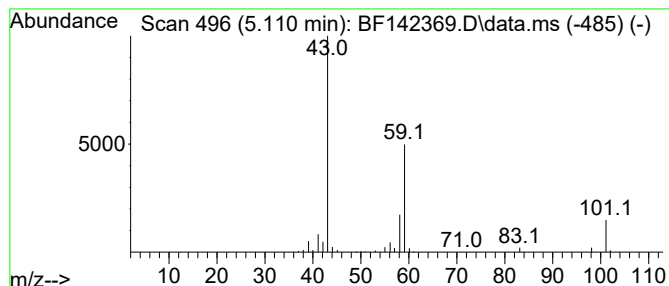
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	9.75 ng	469738	1,4-Dichlorobenzene-d4	6.898

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	23		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
Data File : BF142369.D
Acq On : 14 May 2025 16:46
Operator : RC/JU
Sample : Q2004-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2811

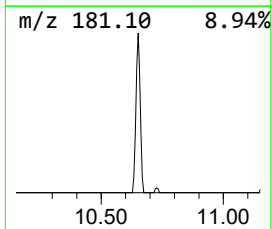
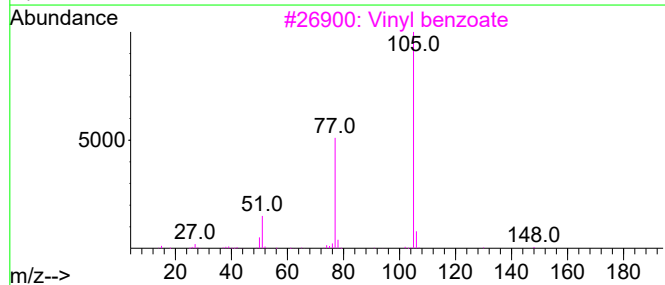
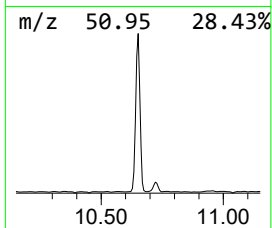
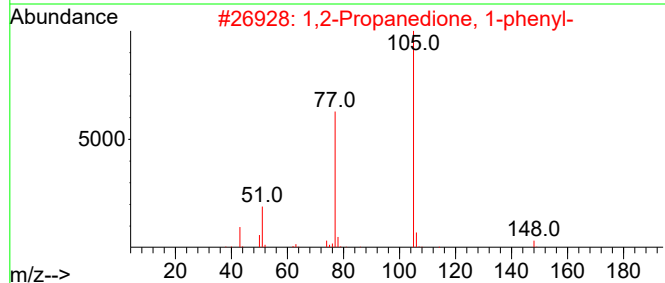
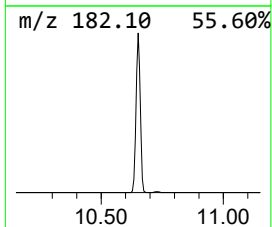
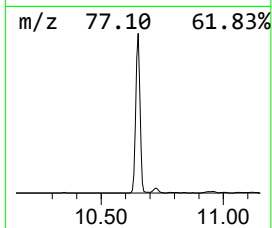
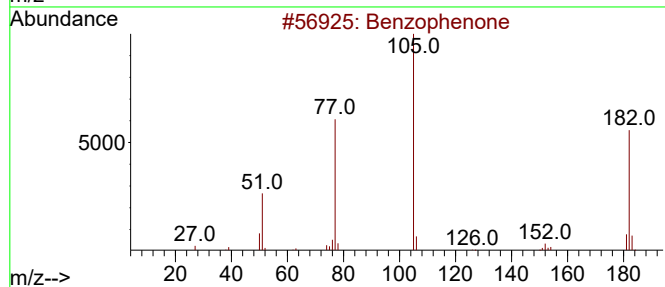
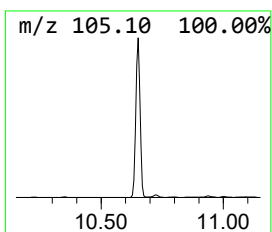
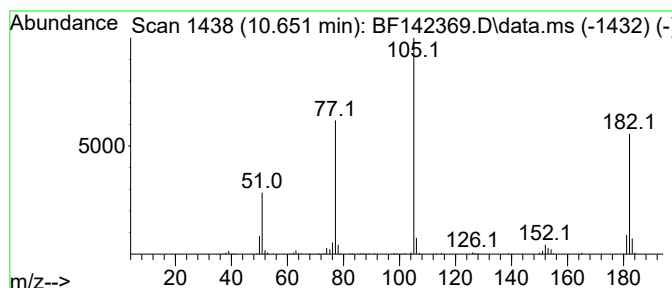
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	4.33 ng	353792	Acenaphthene-d10	9.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
3			Vinyl benzoate	148	C9H8O2	000769-78-8	47
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5			N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
Data File : BF142369.D
Acq On : 14 May 2025 16:46
Operator : RC/JU
Sample : Q2004-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2811

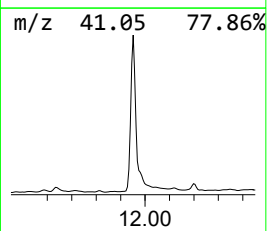
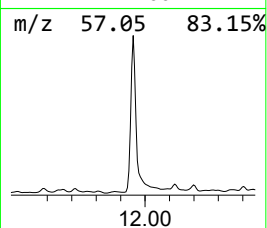
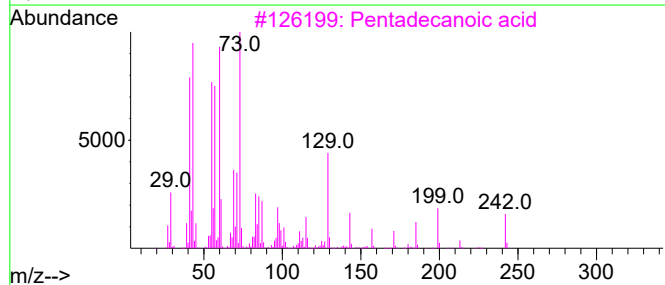
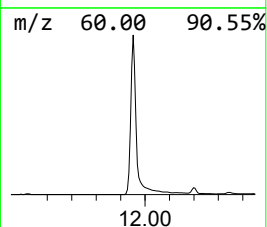
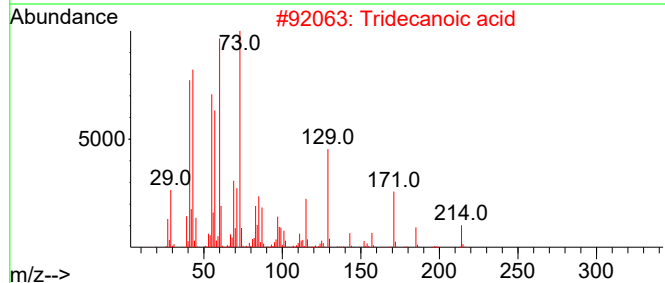
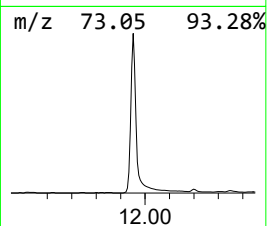
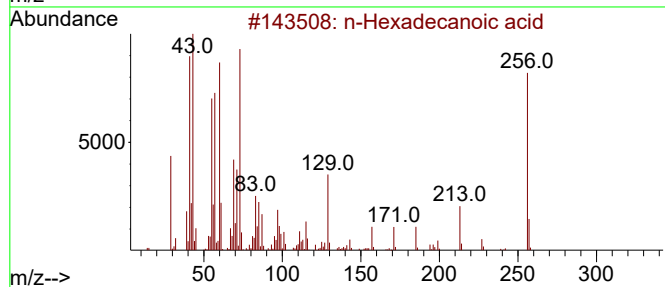
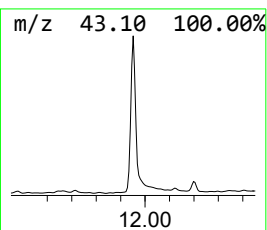
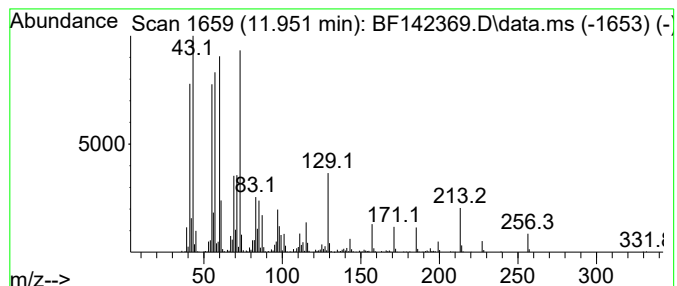
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	13.47 ng	1175060	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Octadecanoic acid	284	C18H36O2	000057-11-4	81
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
Data File : BF142369.D
Acq On : 14 May 2025 16:46
Operator : RC/JU
Sample : Q2004-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2811

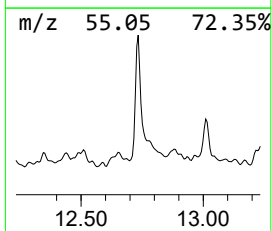
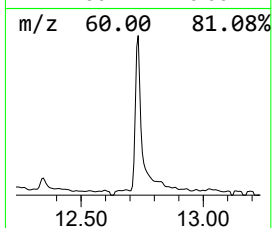
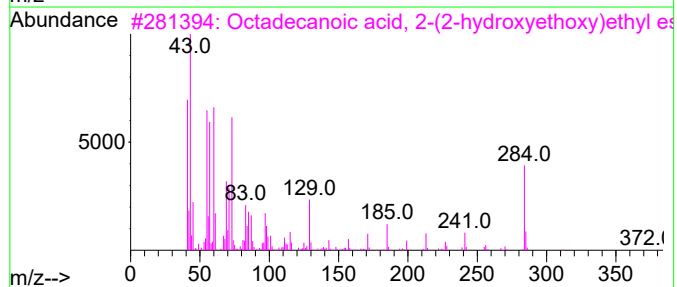
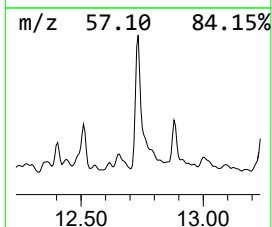
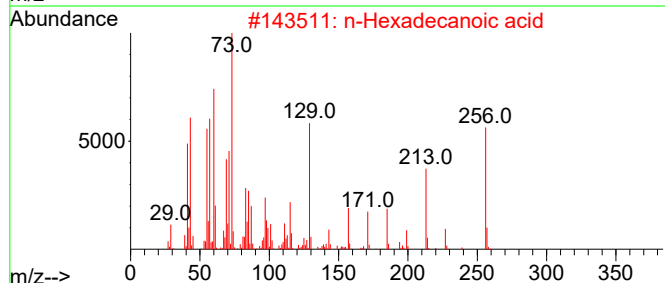
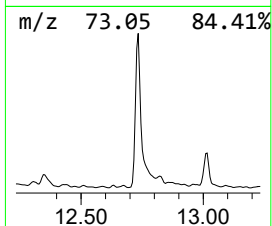
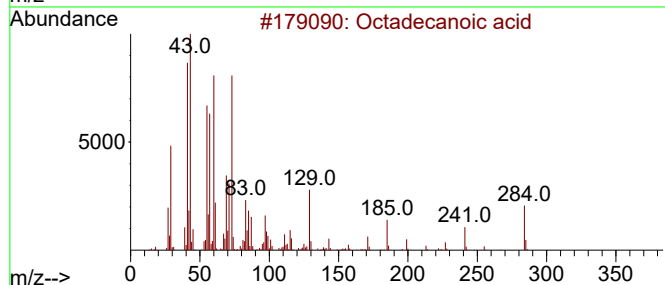
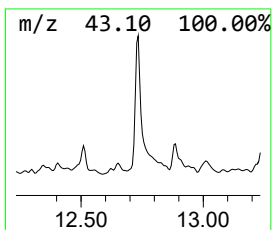
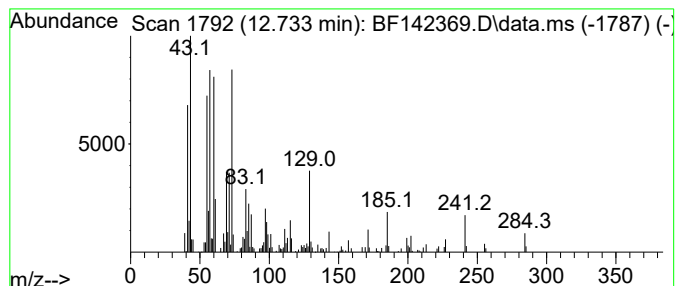
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	2.24 ng	195577	Phenanthrene-d10	11.422

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			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
Data File : BF142369.D
Acq On : 14 May 2025 16:46
Operator : RC/JU
Sample : Q2004-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2811

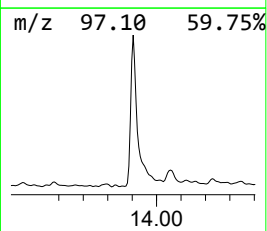
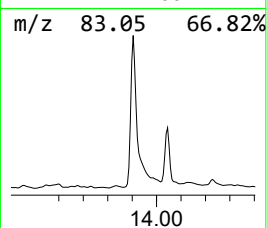
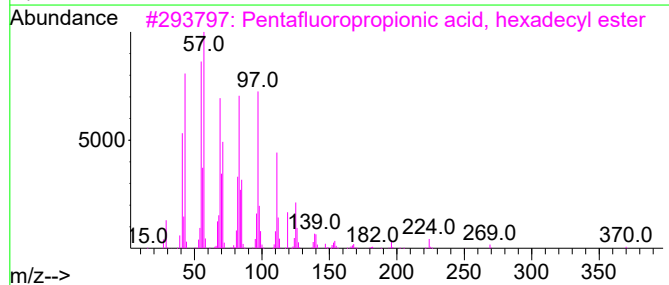
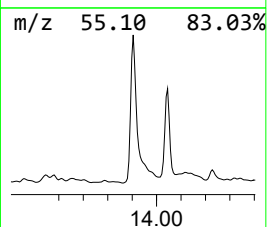
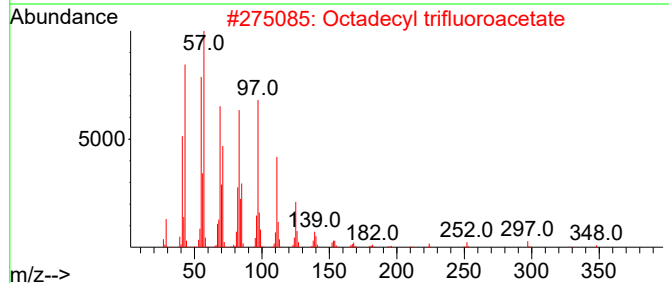
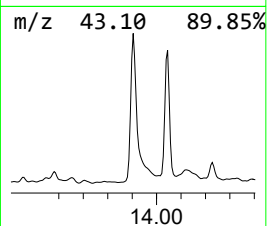
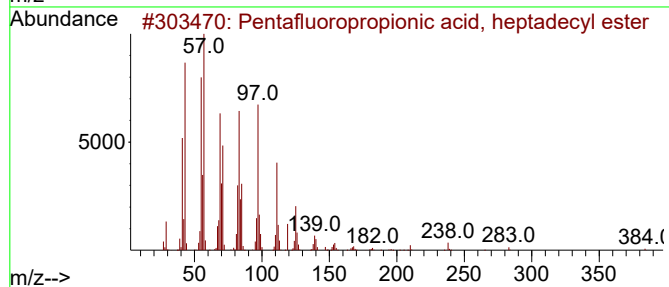
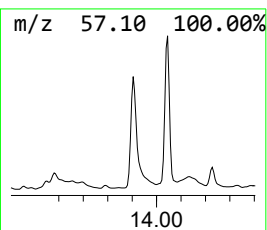
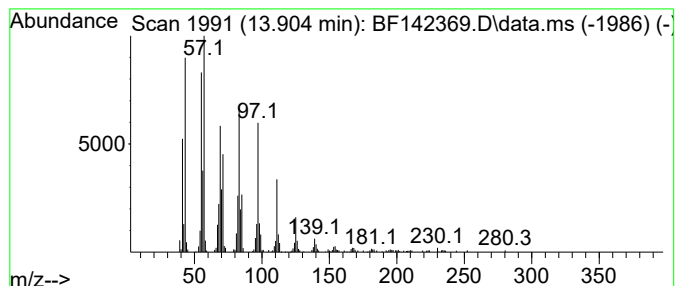
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	4.68 ng	445125	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
2			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
3			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	94
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051425\
Data File : BF142369.D
Acq On : 14 May 2025 16:46
Operator : RC/JU
Sample : Q2004-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
2811

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.110	9.8	ng	469738	1	6.898	963791	20.0
Benzophenone	10.651	4.3	ng	353792	3	9.939	1633740	20.0
n-Hexadecanoic ...	11.951	13.5	ng	1175060	4	11.422	1744450	20.0
Octadecanoic acid	12.733	2.2	ng	195577	4	11.422	1744450	20.0
Pentafluoroprop...	13.904	4.7	ng	445125	5	14.063	1902300	20.0