

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092523\
 Data File : BF135431.D
 Acq On : 25 Sep 2023 17:21
 Operator : CG\JU
 Sample : 04574-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FRAC-TANK-A2421

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135431.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.757	279	284	288	rBV	50992	71812	1.42%	0.252%
2	4.469	401	405	415	rVB	47918	60394	1.19%	0.212%
3	4.981	489	492	498	rVB	46826	53701	1.06%	0.189%
4	5.387	557	561	571	rBV	2331867	2294268	45.27%	8.061%
5	6.392	729	732	752	rVB	1364654	1544725	30.48%	5.428%
6	6.751	789	793	799	rBV	1199893	1008327	19.90%	3.543%
7	7.322	884	890	893	rBV	3148817	3319570	65.50%	11.664%
8	7.428	904	908	912	rVB2	65121	71504	1.41%	0.251%
9	7.563	925	931	941	rVB	132555	175068	3.45%	0.615%
10	8.028	1006	1010	1014	rBV	1373183	1350134	26.64%	4.744%
11	8.316	1056	1059	1064	rVB	143941	138116	2.73%	0.485%
12	9.110	1189	1194	1198	rBV	4744434	5067723	100.00%	17.806%
13	9.227	1210	1214	1217	rVB2	60132	72147	1.42%	0.254%
14	9.786	1303	1309	1313	rBV	1625214	1464652	28.90%	5.146%
15	10.510	1429	1432	1440	rVB	155522	137078	2.70%	0.482%
16	10.586	1440	1445	1448	rBV	2901014	2939417	58.00%	10.328%
17	10.704	1462	1465	1471	rBV2	43435	61387	1.21%	0.216%
18	10.892	1492	1497	1500	rBV3	71459	83994	1.66%	0.295%
19	11.280	1559	1563	1567	rBV	1630668	1379020	27.21%	4.845%
20	11.404	1580	1584	1589	rVB4	30150	52503	1.04%	0.184%
21	11.580	1611	1614	1619	rVB	103027	83795	1.65%	0.294%
22	11.668	1626	1629	1637	rVB3	44081	65886	1.30%	0.232%
23	11.816	1649	1654	1665	rBV2	763155	944080	18.63%	3.317%
24	12.268	1728	1731	1741	rVB	43533	62024	1.22%	0.218%
25	12.527	1769	1775	1780	rBV10	20692	51902	1.02%	0.182%
26	12.604	1785	1788	1799	rVV	250157	317576	6.27%	1.116%
27	12.780	1815	1818	1825	rVB	34572	52167	1.03%	0.183%
28	12.880	1830	1835	1838	rBV	3849559	3734841	73.70%	13.123%
29	13.851	1995	2000	2008	rBV4	82263	199216	3.93%	0.700%
30	13.939	2011	2015	2019	rVB	717662	694132	13.70%	2.439%
31	14.786	2155	2159	2163	rBV	70856	80115	1.58%	0.281%
32	15.398	2259	2263	2277	rVB	602436	828846	16.36%	2.912%

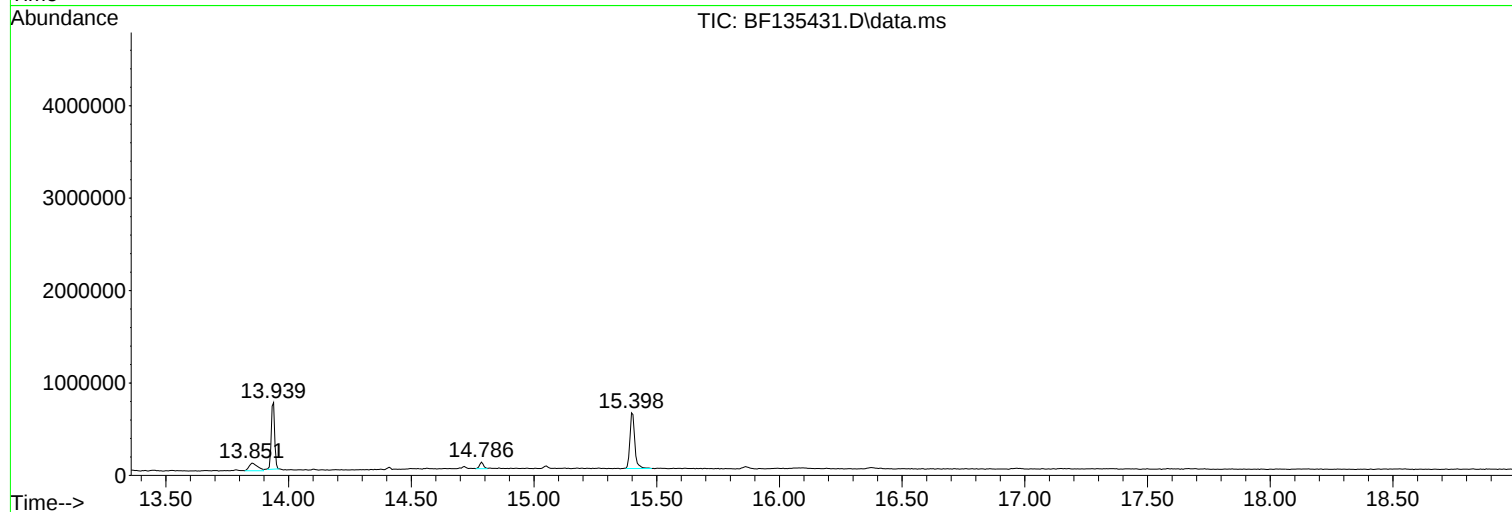
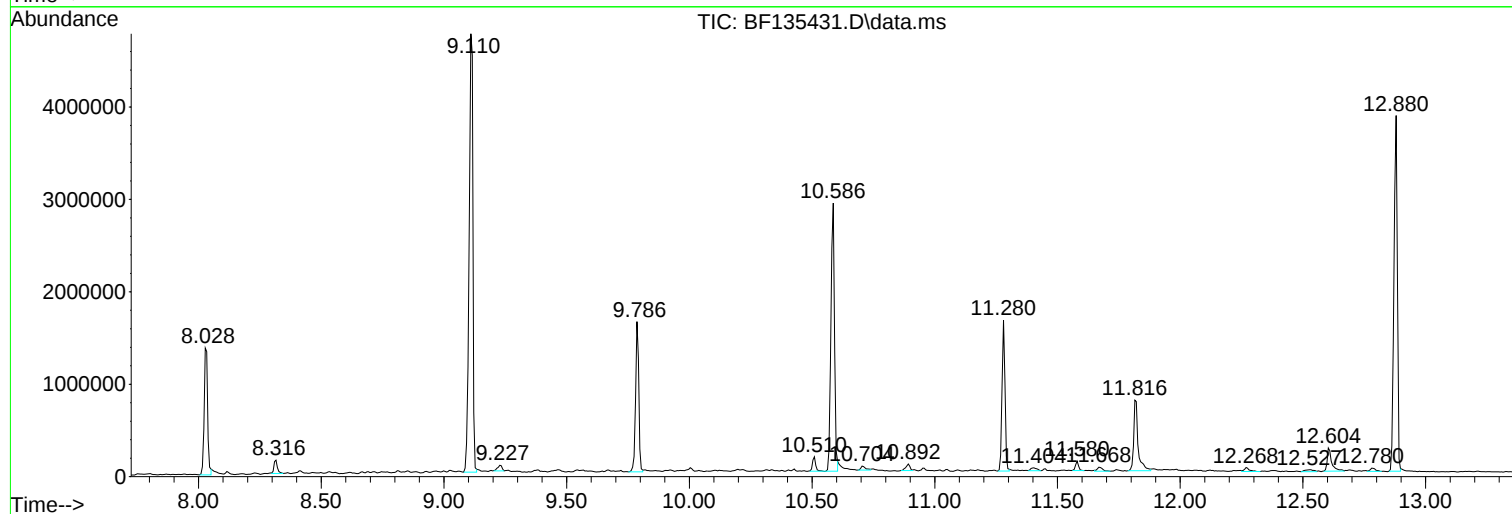
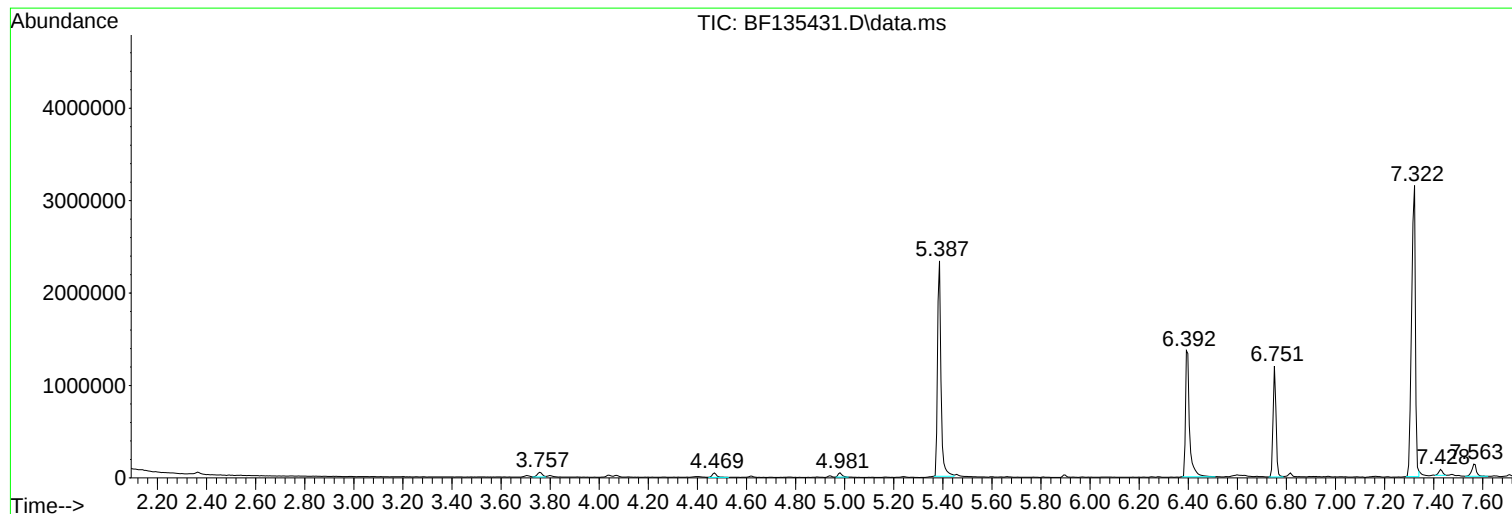
Sum of corrected areas: 28460120

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092523\
Data File : BF135431.D
Acq On : 25 Sep 2023 17:21
Operator : CG\JU
Sample : 04574-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FRAC-TANK-A2421

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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\BF092523\
Data File : BF135431.D
Acq On : 25 Sep 2023 17:21
Operator : CG\JU
Sample : 04574-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

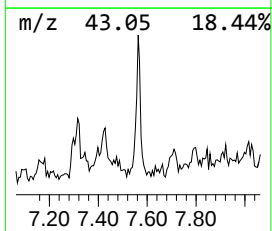
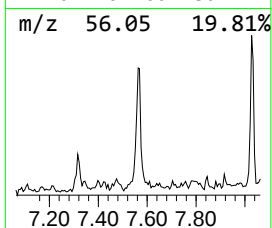
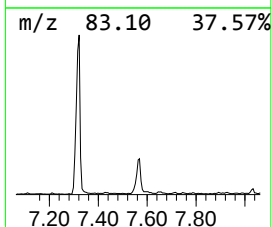
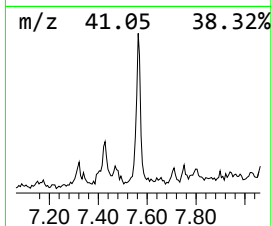
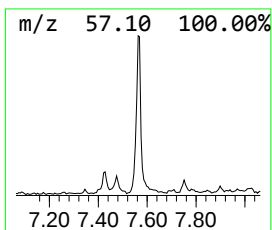
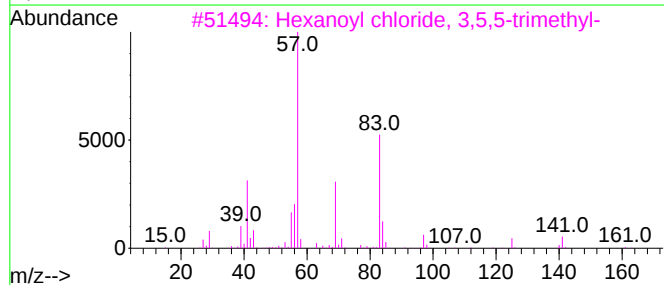
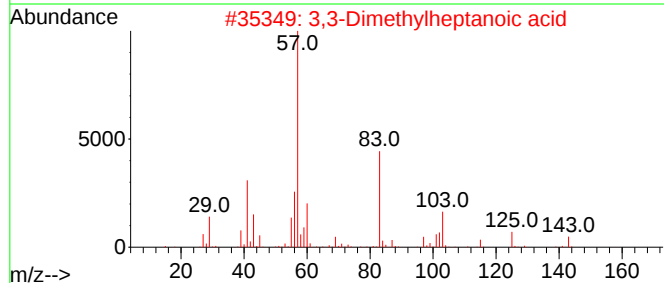
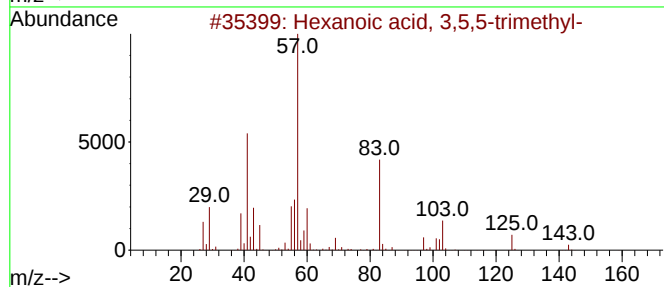
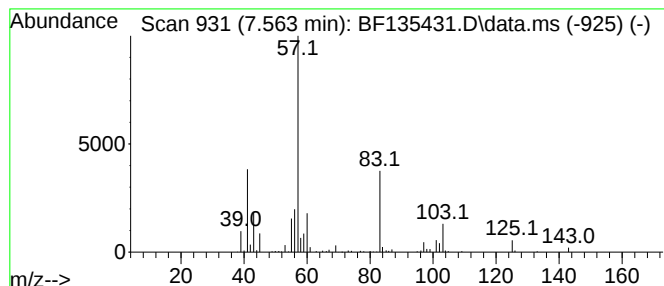
Instrument :
BNA_F
ClientSampleId :
FRAC-TANK-A2421

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexanoic acid, 3,5,5-trimet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
7.563	2.59 ng	175068	Naphthalene-d8	8.033	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	90
2	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	83
3	Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	40
4	Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	25
5	Formic acid, 4,4-dimethylpent-2-...	144	C8H16O2	1000368-69-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092523\
Data File : BF135431.D
Acq On : 25 Sep 2023 17:21
Operator : CG\JU
Sample : 04574-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FRAC-TANK-A2421

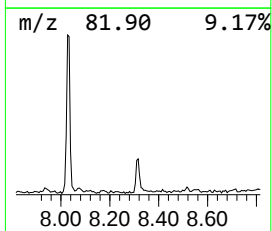
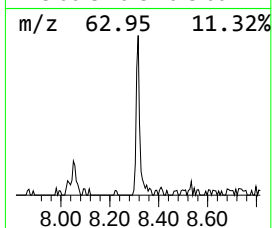
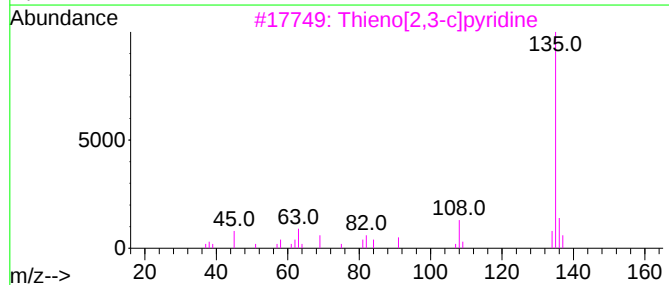
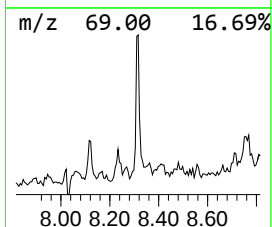
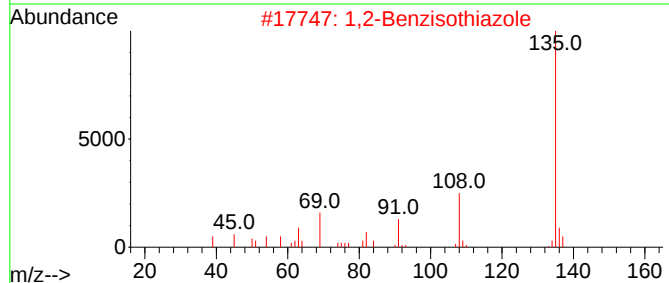
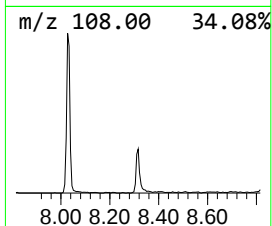
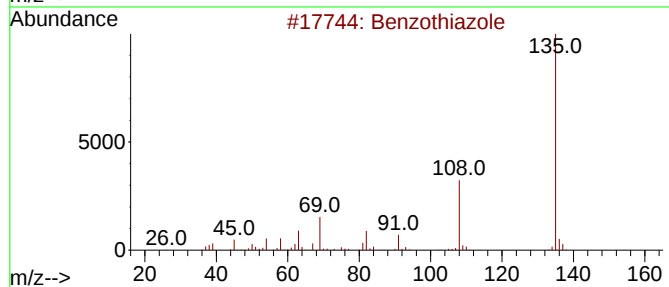
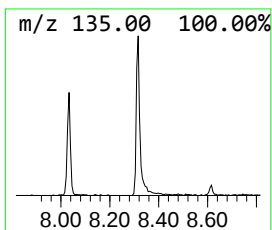
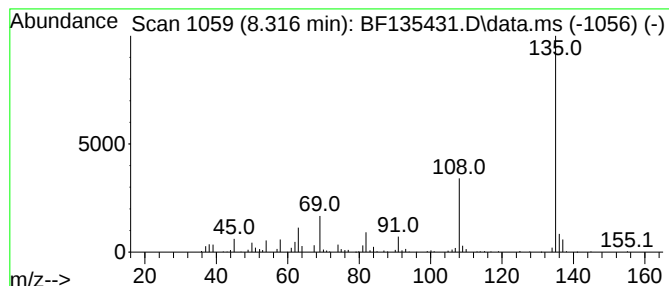
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzothiazole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.316	2.05 ng	138116	Naphthalene-d8	8.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzothiazole	135	C7H5NS	000095-16-9	95
2			1,2-Benzisothiazole	135	C7H5NS	000272-16-2	91
3			Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	64
4			3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	64
5			1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092523\
Data File : BF135431.D
Acq On : 25 Sep 2023 17:21
Operator : CG\JU
Sample : 04574-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FRAC-TANK-A2421

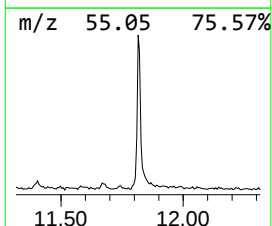
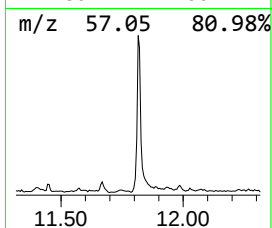
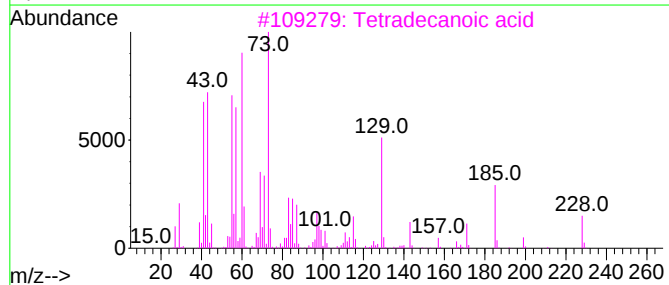
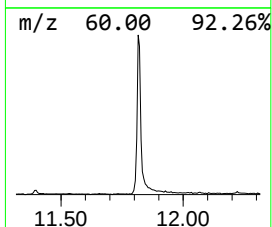
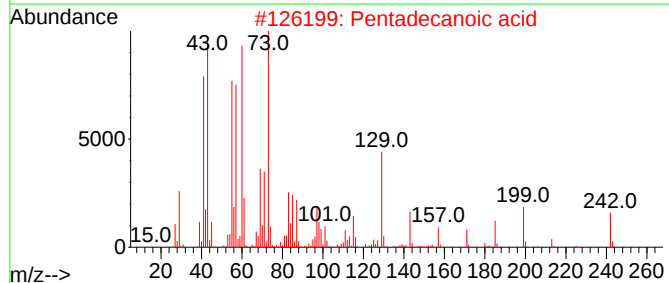
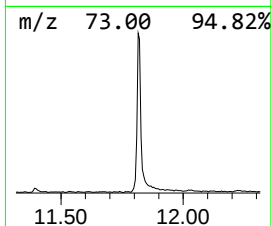
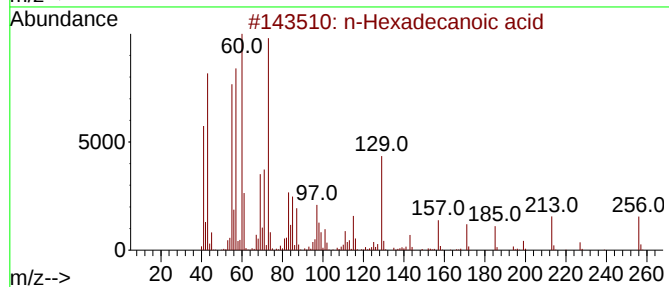
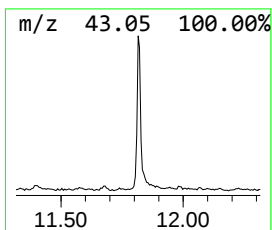
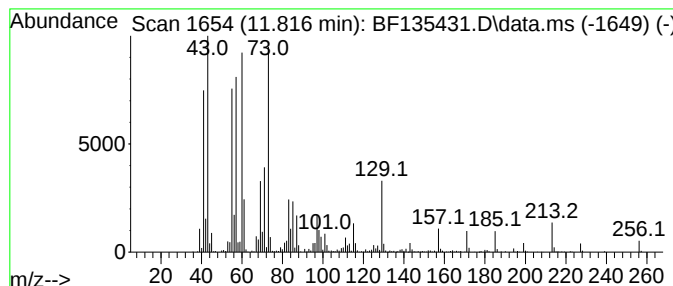
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
11.816	13.69 ng	944080	Phenanthrene-d10	11.280

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	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		Tridecanoic acid	214	C13H26O2	000638-53-9	64
5		Octanoic acid	144	C8H16O2	000124-07-2	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092523\
Data File : BF135431.D
Acq On : 25 Sep 2023 17:21
Operator : CG\JU
Sample : 04574-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FRAC-TANK-A2421

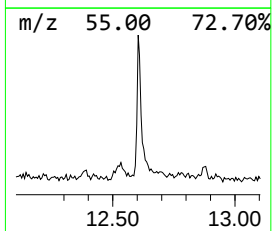
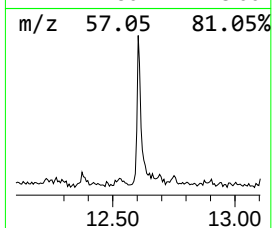
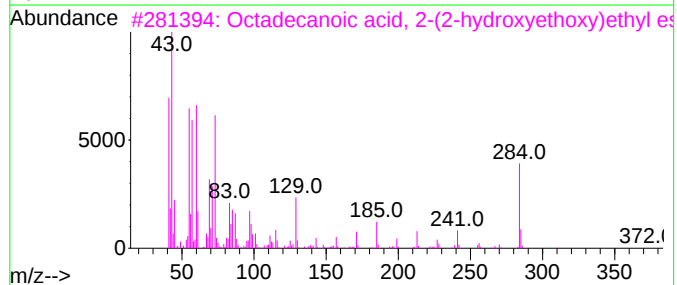
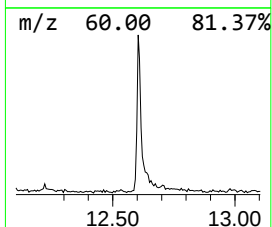
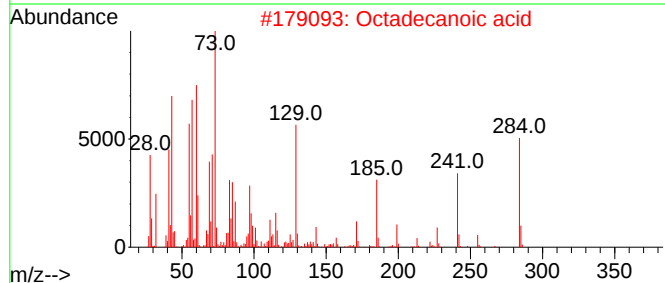
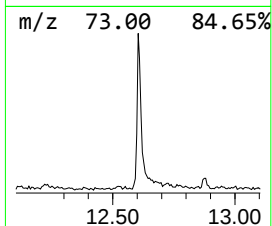
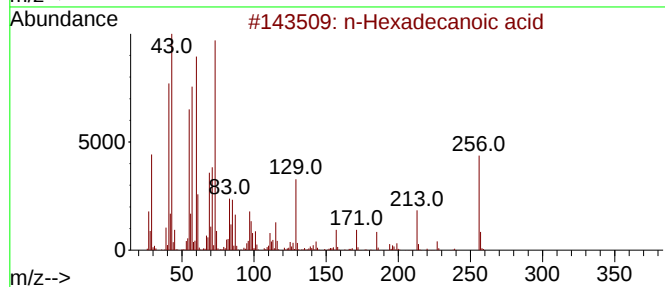
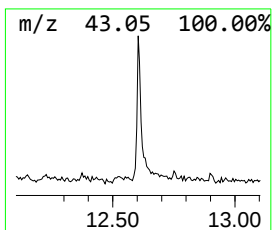
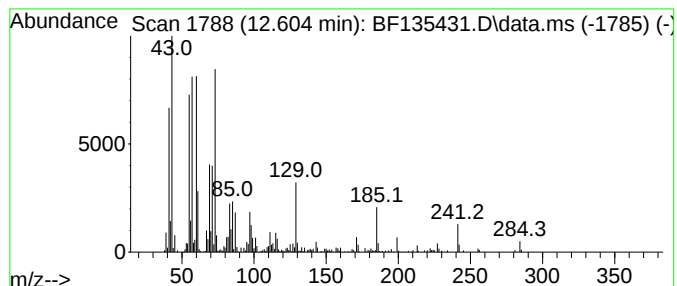
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.604	4.61 ng	317576	Phenanthrene-d10	11.280

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Octadecanoic acid	284	C18H36O2	000057-11-4	93
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5			Undecanoic acid	186	C11H22O2	000112-37-8	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092523\
Data File : BF135431.D
Acq On : 25 Sep 2023 17:21
Operator : CG\JU
Sample : 04574-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FRAC-TANK-A2421

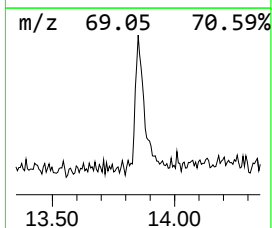
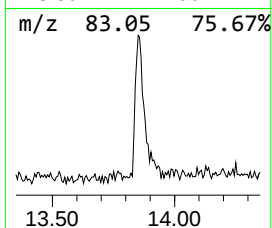
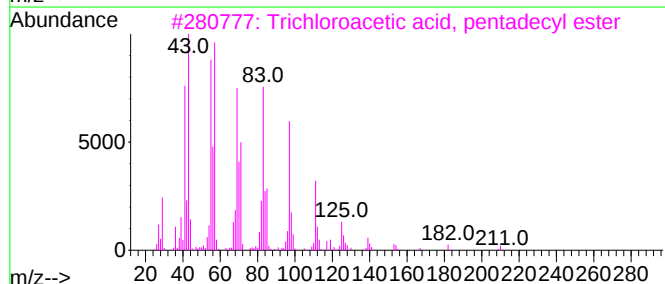
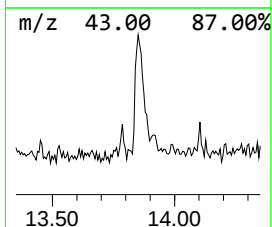
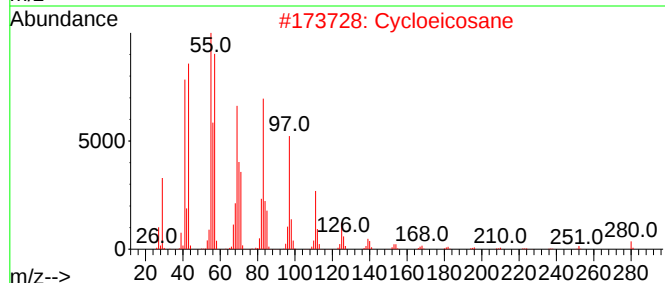
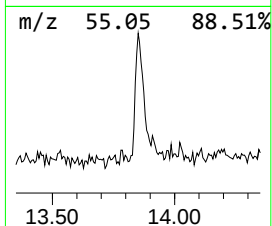
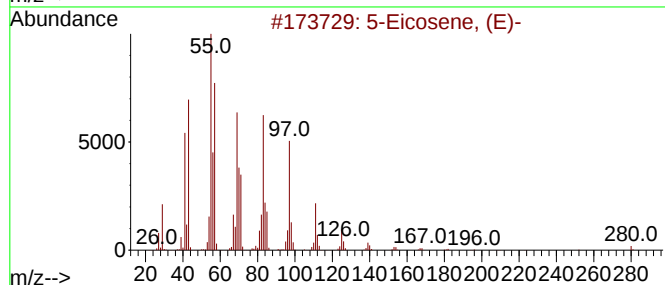
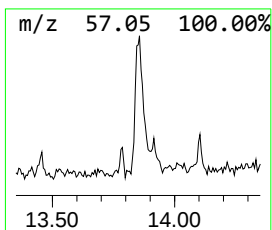
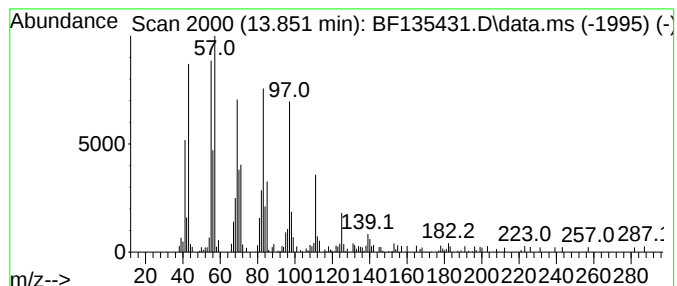
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	5.74 ng	199216	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Eicosene, (E)-	280	C20H40	074685-30-6	91
2			Cycloeicosane	280	C20H40	000296-56-0	91
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092523\
Data File : BF135431.D
Acq On : 25 Sep 2023 17:21
Operator : CG\JU
Sample : 04574-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FRAC-TANK-A2421

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
Hexanoic acid, ...	7.563	2.6	ng	175068	2	8.033	1350130	20.0
Benzothiazole	8.316	2.0	ng	138116	2	8.033	1350130	20.0
n-Hexadecanoic ...	11.816	13.7	ng	944080	4	11.280	1379020	20.0
Octadecanoic acid	12.604	4.6	ng	317576	4	11.280	1379020	20.0
5-Eicosene, (E)-	13.851	5.7	ng	199216	5	13.939	694132	20.0