

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
 Data File : BF136968.D
 Acq On : 05 Jan 2024 10:47
 Operator : CG\JU
 Sample : PB158239BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB158239BL

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136968.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	16	rVB	28830	39436	1.12%	0.191%
2	5.069	502	507	519	rVB	48500	86588	2.47%	0.420%
3	5.445	566	571	574	rBV	2701454	2759314	78.71%	13.385%
4	6.445	735	741	744	rBV	2418479	2745684	78.32%	13.319%
5	6.781	795	798	802	rBV	570184	513618	14.65%	2.491%
6	7.351	889	895	898	rBV	1654469	1876992	53.54%	9.105%
7	8.057	1011	1015	1019	rBV	716957	684421	19.52%	3.320%
8	9.145	1193	1200	1202	rBV	3274780	3505678	100.00%	17.005%
9	9.816	1309	1314	1318	rBV	892854	771064	21.99%	3.740%
10	10.616	1445	1450	1454	rBV	1811487	1976267	56.37%	9.586%
11	11.310	1564	1568	1572	rBV	902572	818603	23.35%	3.971%
12	12.915	1835	1841	1844	rBV	3326424	3441035	98.16%	16.692%
13	13.968	2016	2020	2032	rVB	583845	558194	15.92%	2.708%
14	14.745	2148	2152	2156	rVB3	32799	38296	1.09%	0.186%
15	15.086	2207	2210	2217	rVB	37133	45149	1.29%	0.219%
16	15.456	2268	2273	2283	rVB	326200	514785	14.68%	2.497%
17	15.927	2348	2353	2359	rVB	39965	60883	1.74%	0.295%
18	16.445	2437	2441	2448	rVB2	38289	66488	1.90%	0.323%
19	17.068	2542	2547	2553	rVB3	27443	53506	1.53%	0.260%
20	17.798	2664	2671	2680	rVB6	21407	59491	1.70%	0.289%

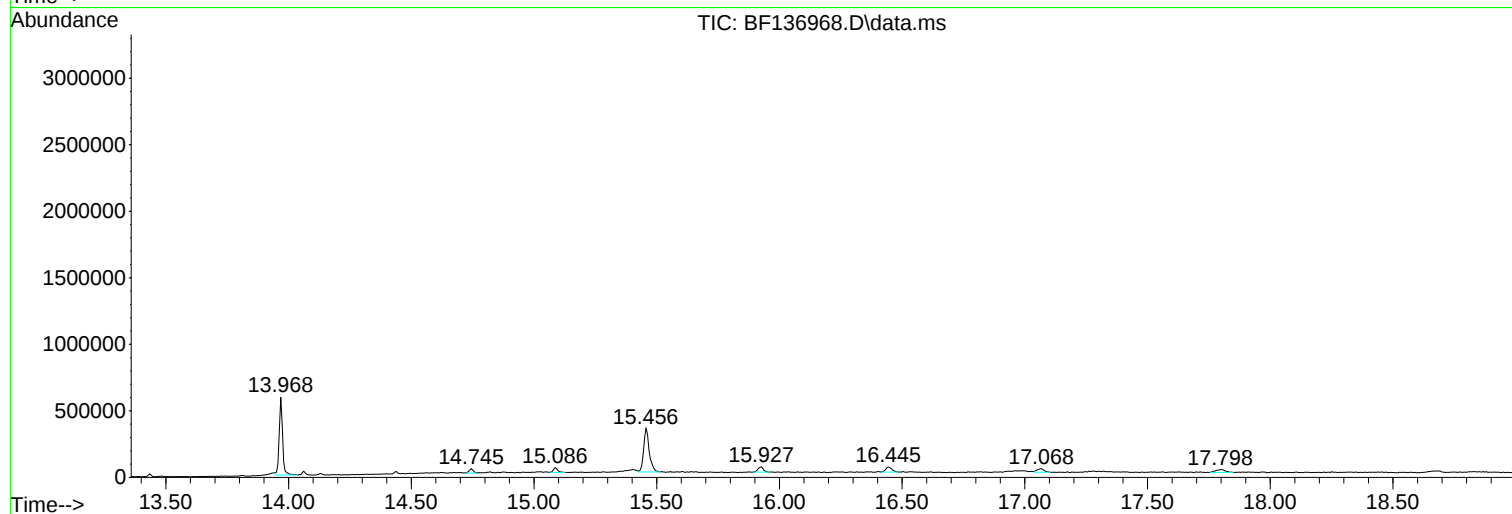
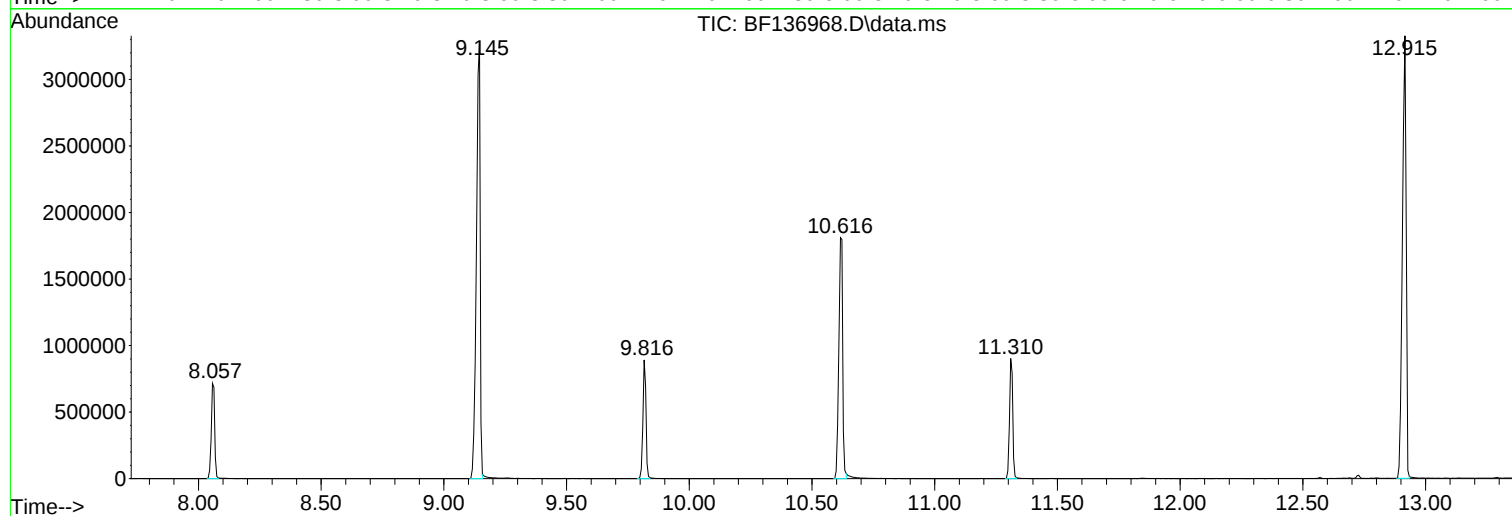
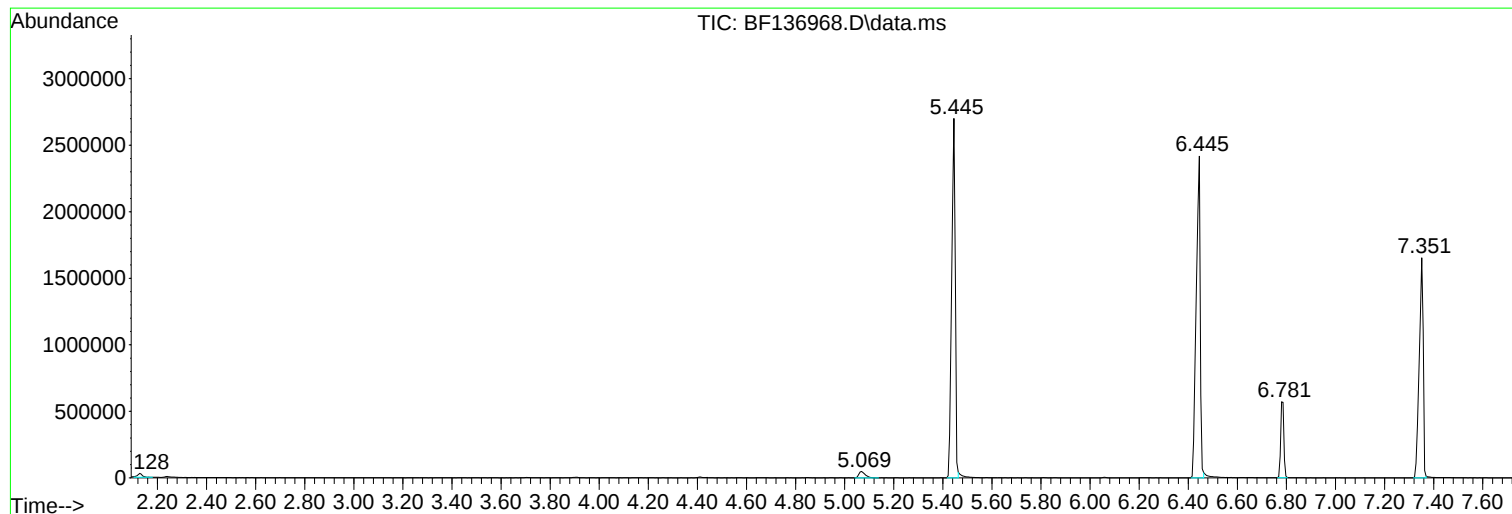
Sum of corrected areas: 20615492

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136968.D
Acq On : 05 Jan 2024 10:47
Operator : CG\JU
Sample : PB158239BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158239BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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\BF010524\
Data File : BF136968.D
Acq On : 05 Jan 2024 10:47
Operator : CG\JU
Sample : PB158239BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158239BL

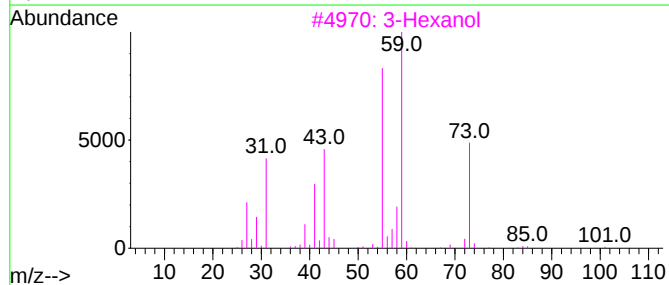
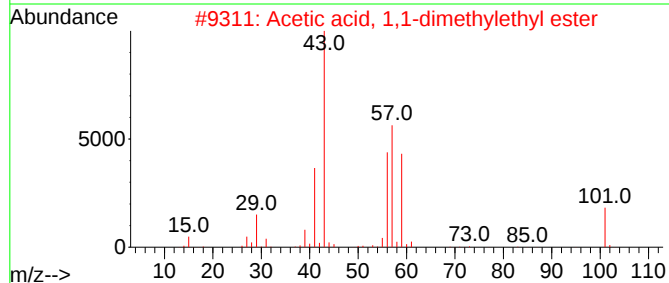
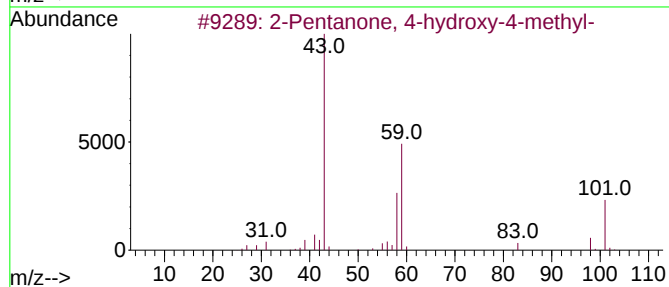
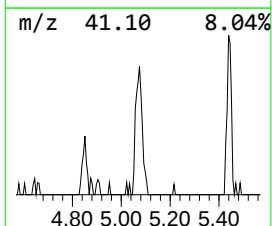
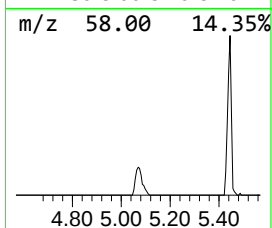
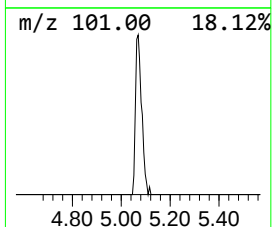
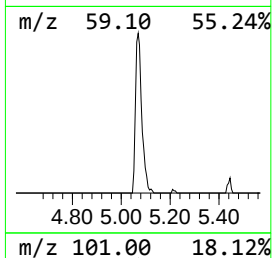
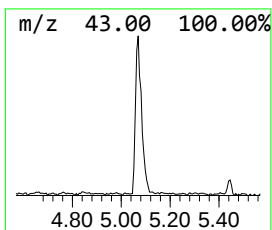
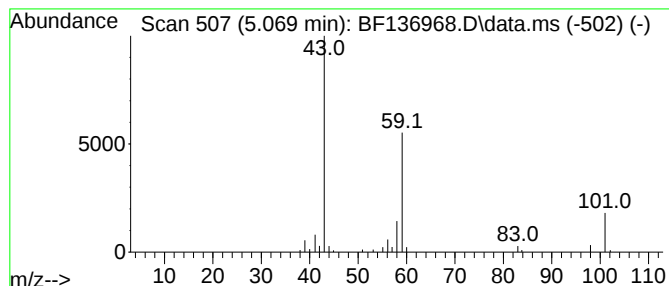
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown5.069 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	3.37 ng	86588	1,4-Dichlorobenzene-d4	6.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	3-Hexanol	102	C6H14O	000623-37-0	33		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136968.D
Acq On : 05 Jan 2024 10:47
Operator : CG\JU
Sample : PB158239BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158239BL

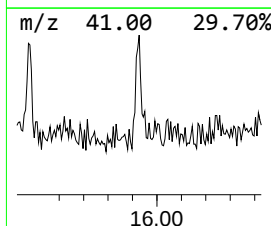
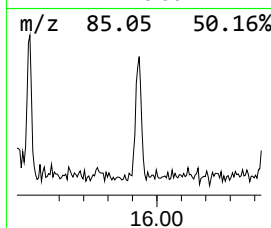
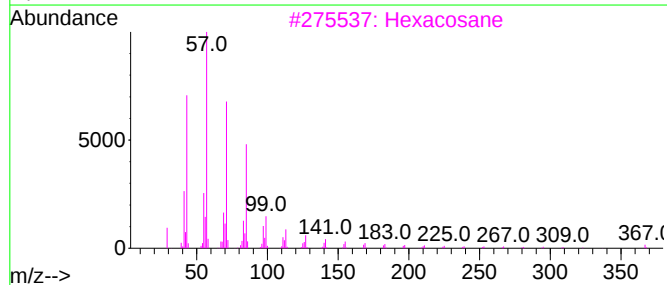
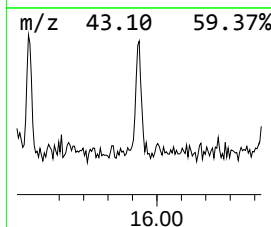
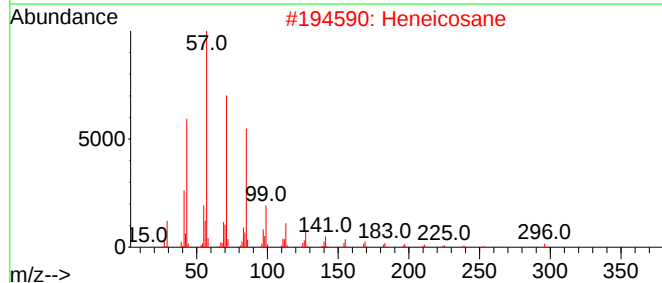
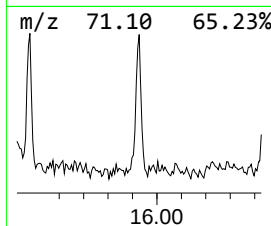
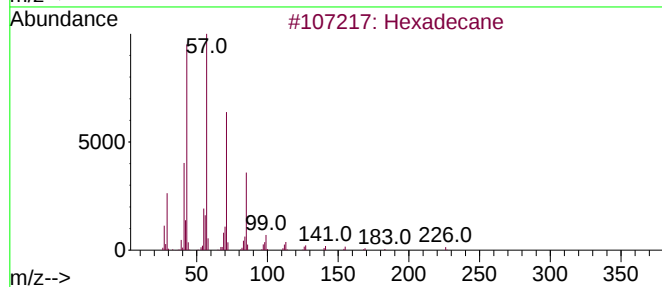
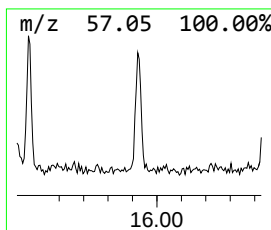
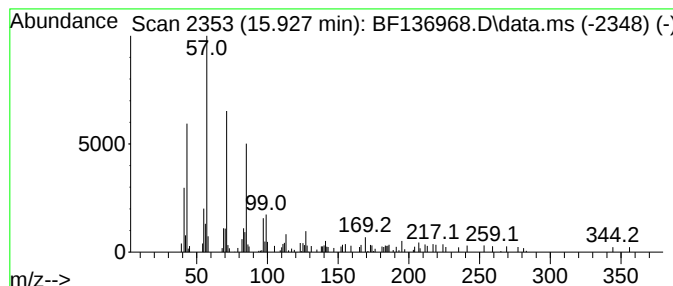
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.927	2.37 ng	60883	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	95
2			Heneicosane	296	C21H44	000629-94-7	87
3			Hexacosane	366	C26H54	000630-01-3	87
4			Pentacosane	352	C25H52	000629-99-2	87
5			Octadecane	254	C18H38	000593-45-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136968.D
Acq On : 05 Jan 2024 10:47
Operator : CG\JU
Sample : PB158239BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158239BL

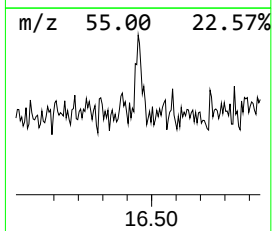
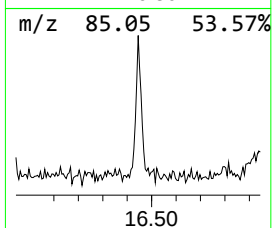
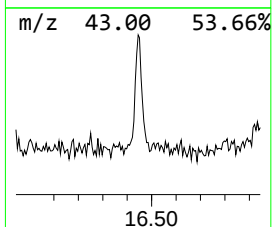
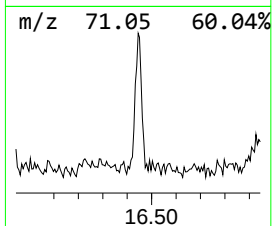
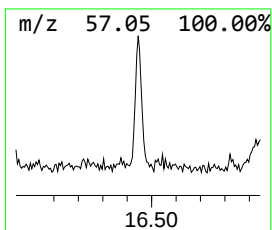
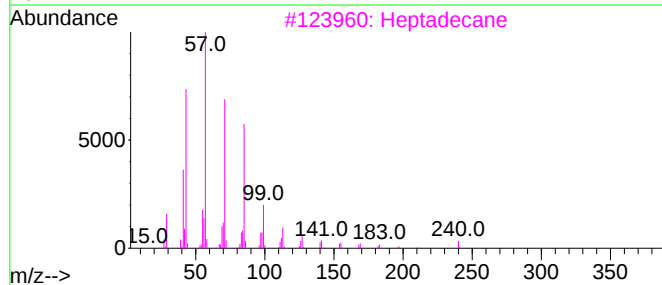
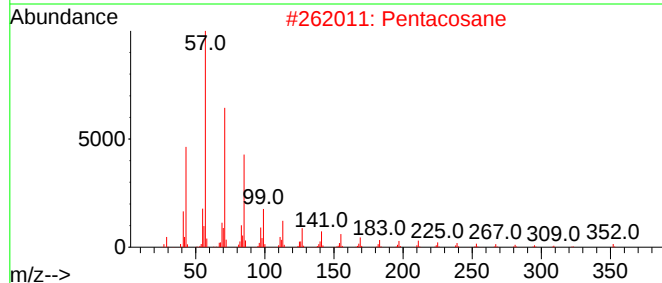
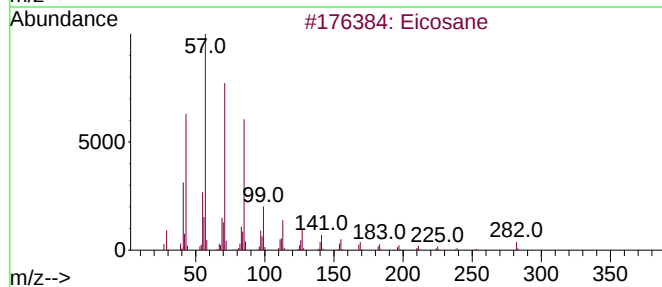
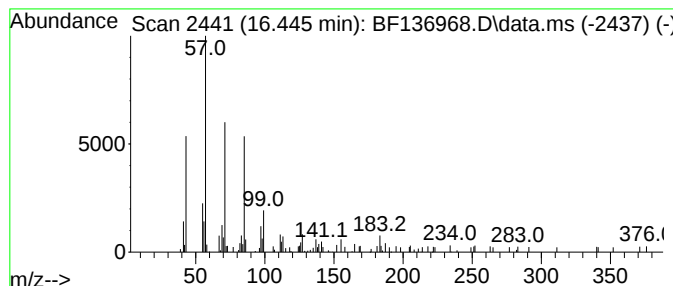
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Eicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.445	2.58 ng	66488	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	86
2	Pentacosane			352	C25H52	000629-99-2	86
3	Heptadecane			240	C17H36	000629-78-7	80
4	Tetracosane			338	C24H50	000646-31-1	80
5	Eicosane, 1-iodo-			408	C20H41I	1000406-31-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136968.D
Acq On : 05 Jan 2024 10:47
Operator : CG\JU
Sample : PB158239BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158239BL

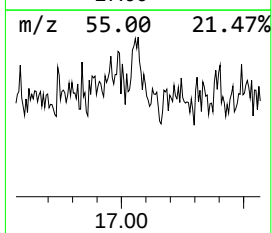
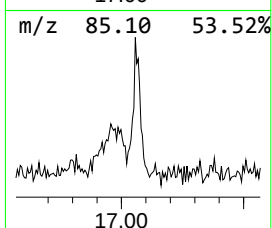
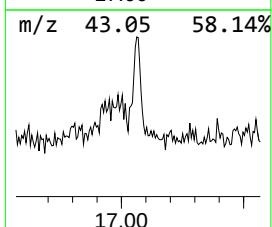
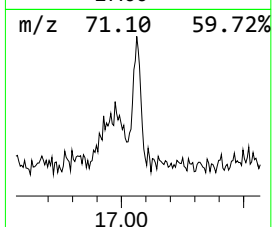
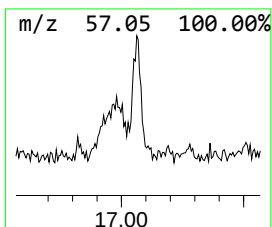
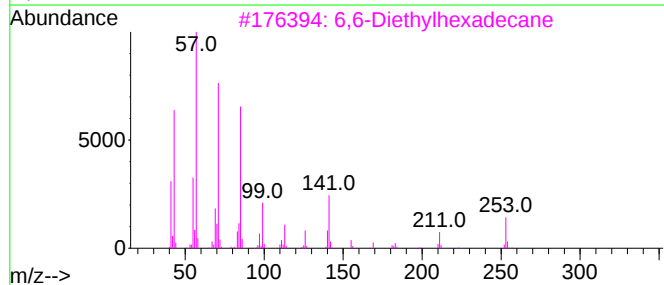
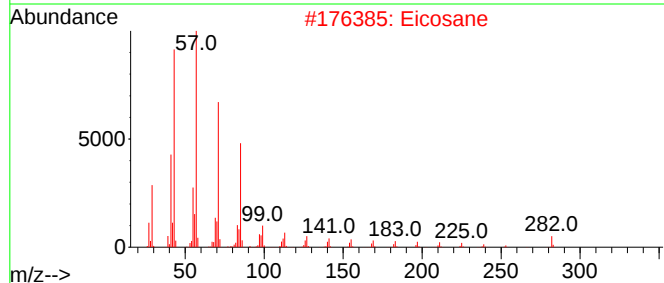
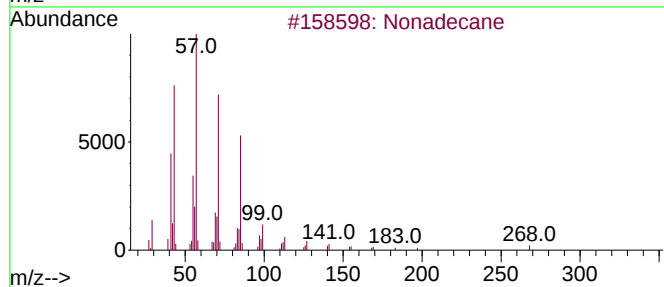
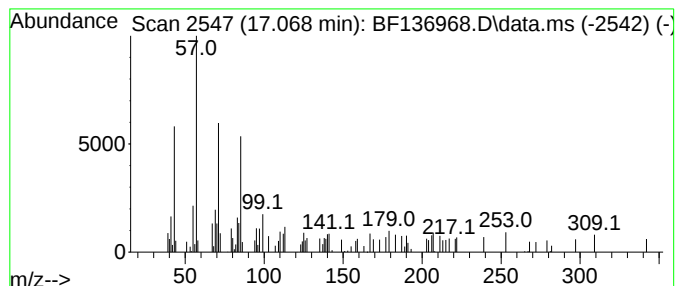
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.068	2.08 ng	53506	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	64
2			Eicosane	282	C20H42	000112-95-8	60
3			6,6-Diethylhexadecane	282	C20H42	1000360-41-4	58
4			Docosane, 11-decyl-	451	C32H66	055401-55-3	52
5			2-Methyltetracosane	352	C25H52	001560-78-7	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136968.D
Acq On : 05 Jan 2024 10:47
Operator : CG\JU
Sample : PB158239BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158239BL

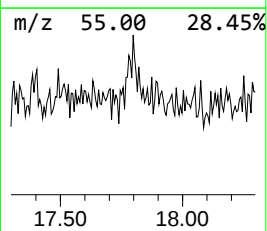
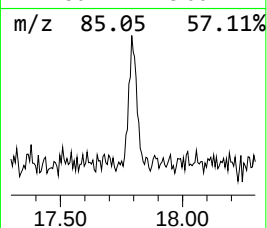
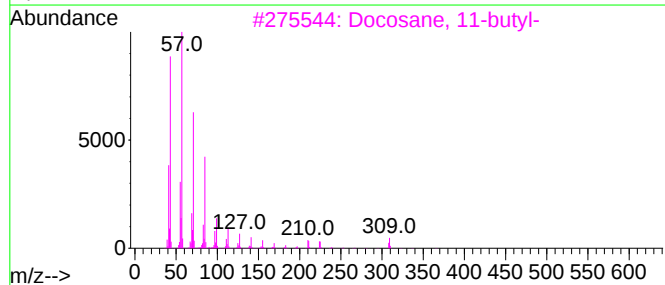
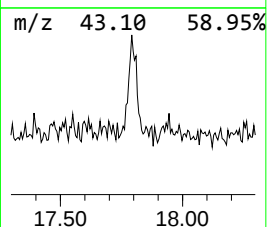
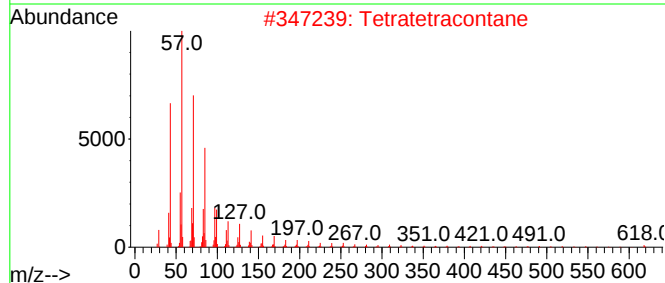
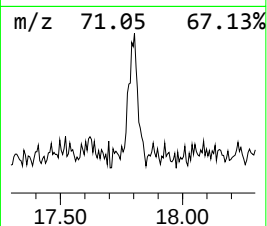
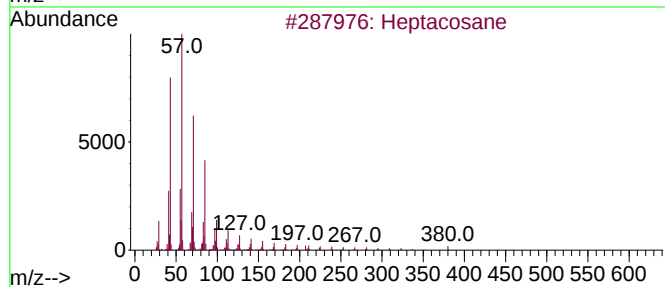
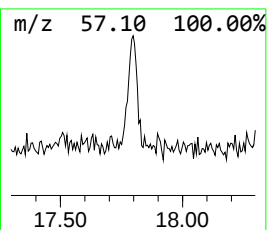
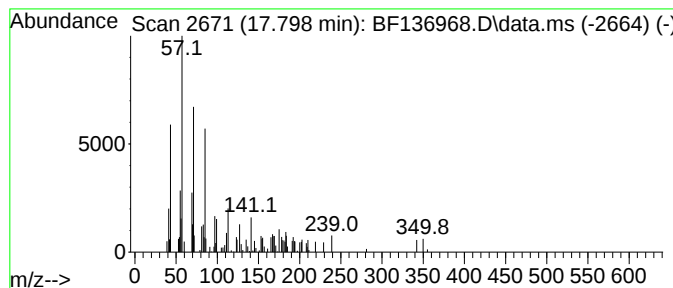
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.797	2.31 ng	59491	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	53
2			Tetratetracontane	619	C44H90	007098-22-8	52
3			Docosane, 11-butyl-	366	C26H54	013475-76-8	52
4			Heneicosane	296	C21H44	000629-94-7	50
5			Triacontane	422	C30H62	000638-68-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010524\
Data File : BF136968.D
Acq On : 05 Jan 2024 10:47
Operator : CG\JU
Sample : PB158239BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158239BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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
unknown5.069	5.069	3.4	ng	86588	1	6.786	513618	20.0
Hexadecane	15.927	2.4	ng	60883	6	15.457	514785	20.0
Eicosane	16.445	2.6	ng	66488	6	15.457	514785	20.0
Nonadecane	17.068	2.1	ng	53506	6	15.457	514785	20.0
Heptacosane	17.797	2.3	ng	59491	6	15.457	514785	20.0