

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010824\
 Data File : BF136993.D
 Acq On : 08 Jan 2024 12:41
 Operator : CG\JU
 Sample : PB158263BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB158263BL

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: BF136993.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	502	506	518	rBV	43327	74722	2.15%	0.382%
2	5.445	566	571	574	rBV	2462851	2567524	73.89%	13.116%
3	6.445	735	741	743	rBV	2233798	2563541	73.78%	13.096%
4	6.781	795	798	802	rBV	546972	465550	13.40%	2.378%
5	7.351	889	895	898	rBV	1577989	1727574	49.72%	8.825%
6	8.057	1011	1015	1019	rBV	696103	625216	17.99%	3.194%
7	9.145	1193	1200	1202	rBV	3015971	3276870	94.30%	16.740%
8	9.816	1309	1314	1318	rBV	850304	721197	20.76%	3.684%
9	10.616	1445	1450	1467	rBV	1756643	1888802	54.36%	9.649%
10	11.310	1564	1568	1572	rBV	935455	787046	22.65%	4.021%
11	12.916	1835	1841	1844	rBV	3280578	3474765	100.00%	17.751%
12	13.968	2016	2020	2034	rVB	612760	580371	16.70%	2.965%
13	14.745	2147	2152	2155	rBV	34100	39735	1.14%	0.203%
14	15.086	2206	2210	2214	rVB	41877	44930	1.29%	0.230%
15	15.457	2267	2273	2284	rBV	320923	498372	14.34%	2.546%
16	15.921	2345	2352	2357	rBV	40943	68219	1.96%	0.348%
17	16.439	2435	2440	2449	rVB2	35791	64794	1.86%	0.331%
18	17.056	2540	2545	2555	rVB2	23512	48129	1.39%	0.246%
19	17.786	2659	2669	2675	rBV5	20914	58176	1.67%	0.297%

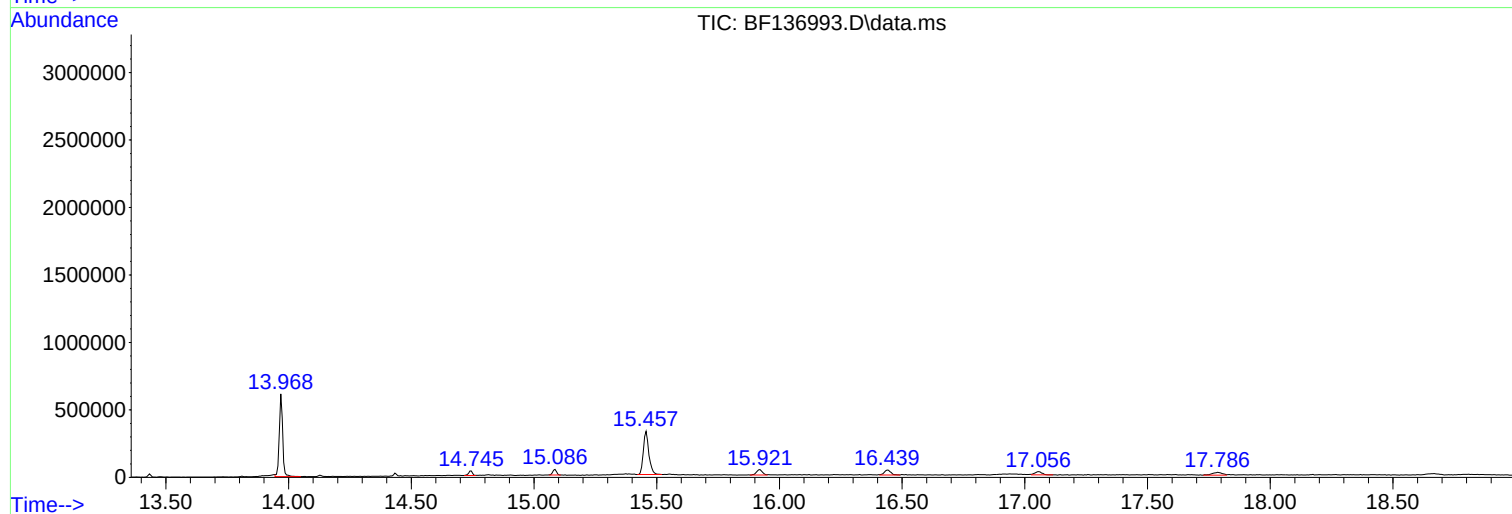
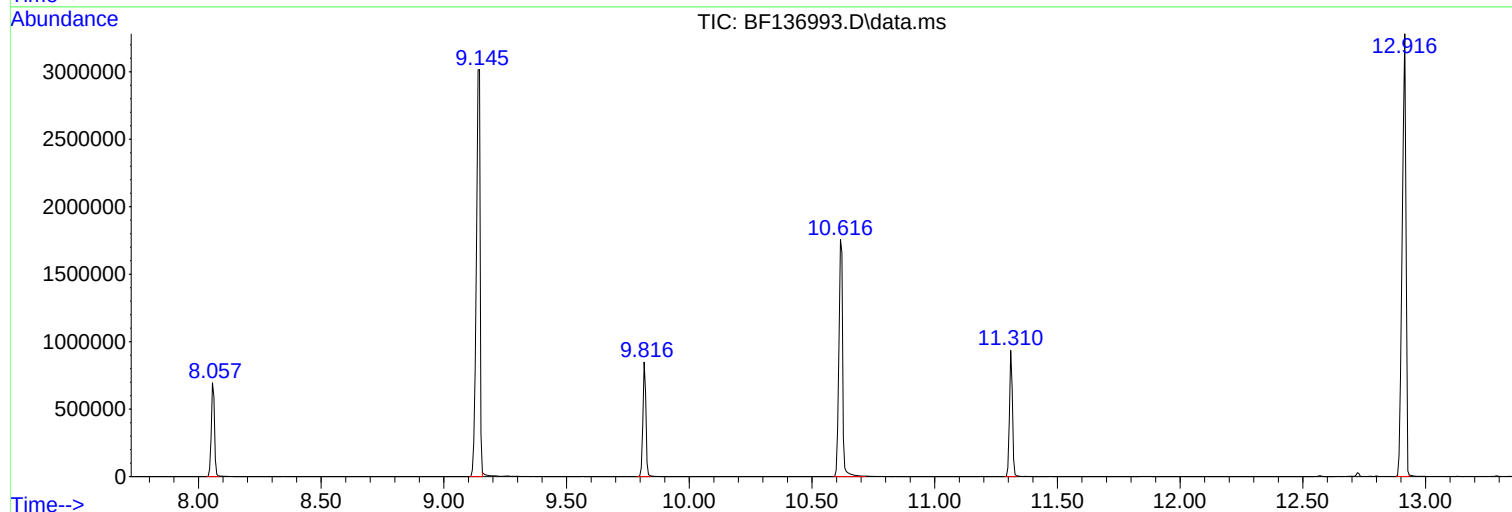
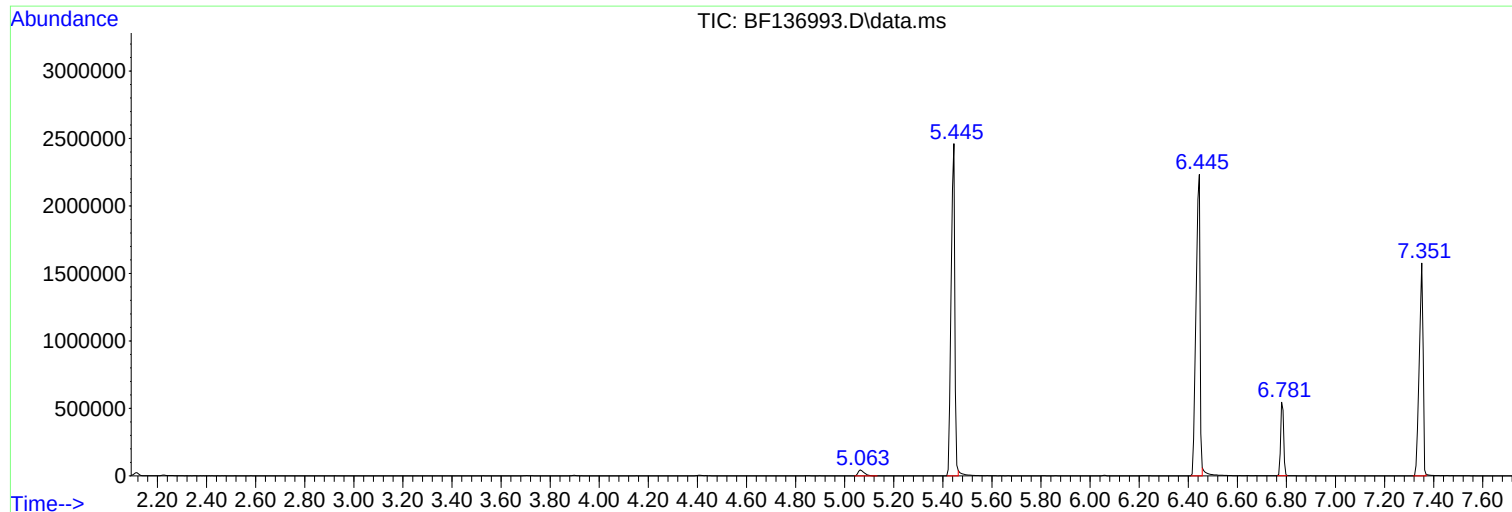
Sum of corrected areas: 19575533

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010824\
Data File : BF136993.D
Acq On : 08 Jan 2024 12:41
Operator : CG\JU
Sample : PB158263BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158263BL

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\BF010824\
Data File : BF136993.D
Acq On : 08 Jan 2024 12:41
Operator : CG\JU
Sample : PB158263BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158263BL

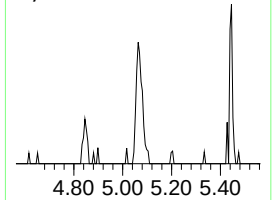
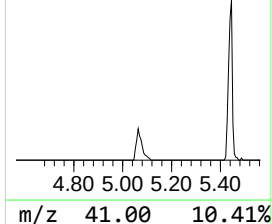
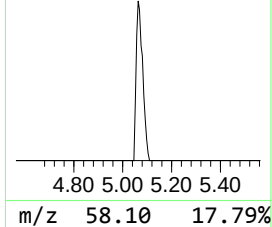
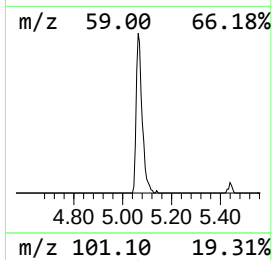
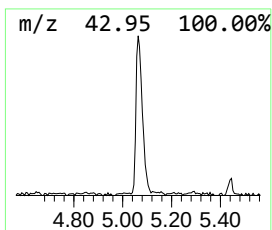
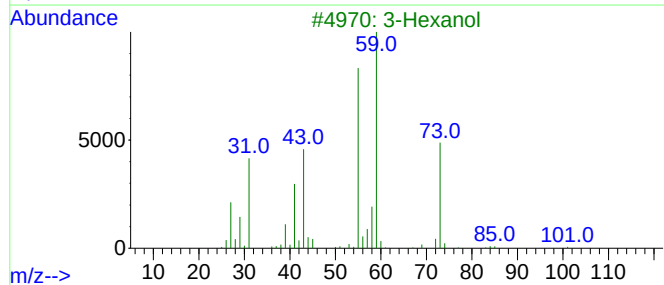
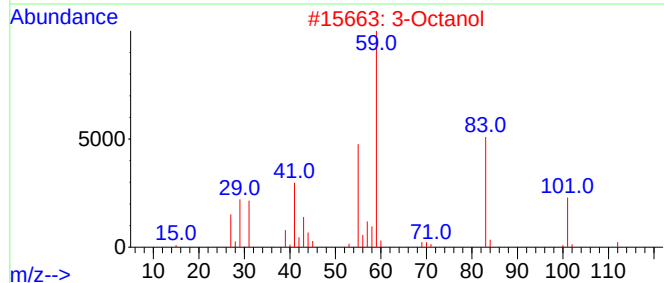
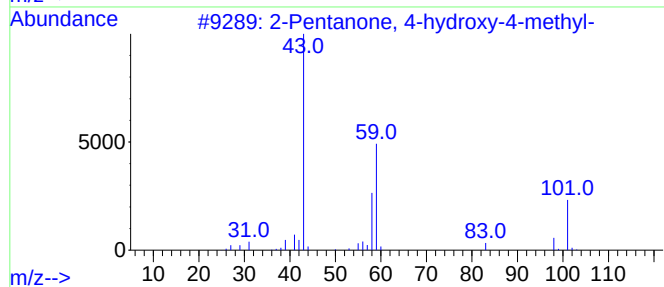
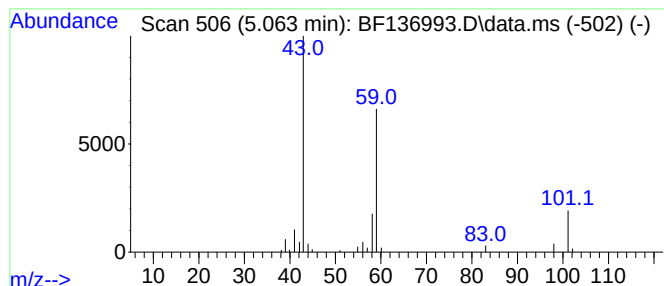
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	3.21 ng	74722	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	3-Octanol	130	C8H18O	000589-98-0	36		
3	3-Hexanol	102	C6H14O	000623-37-0	28		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010824\
Data File : BF136993.D
Acq On : 08 Jan 2024 12:41
Operator : CG\JU
Sample : PB158263BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158263BL

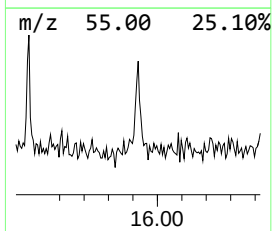
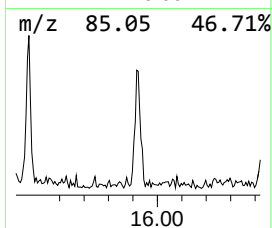
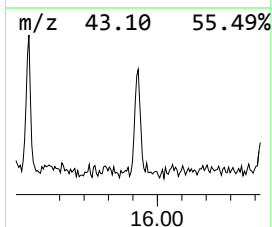
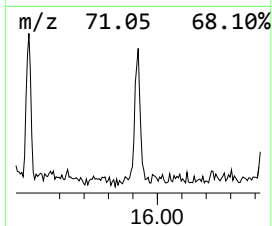
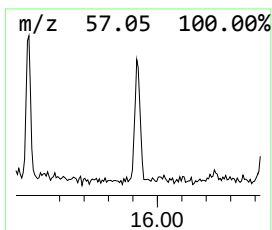
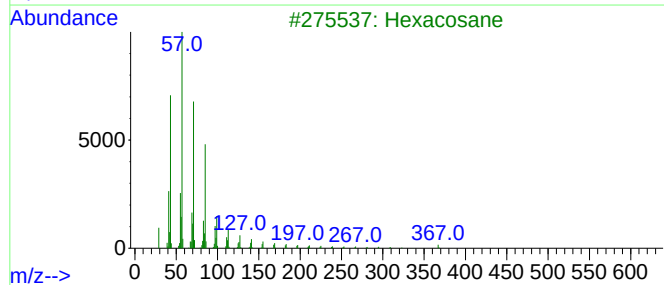
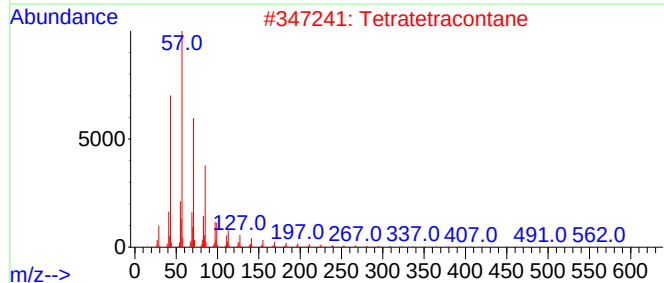
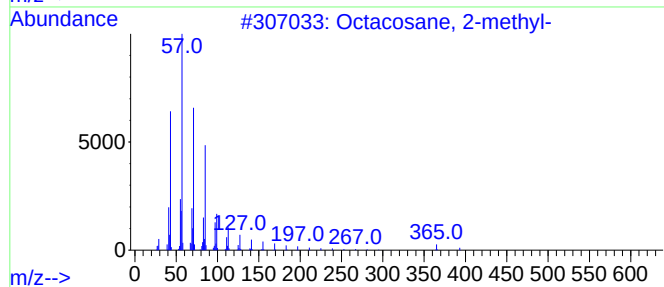
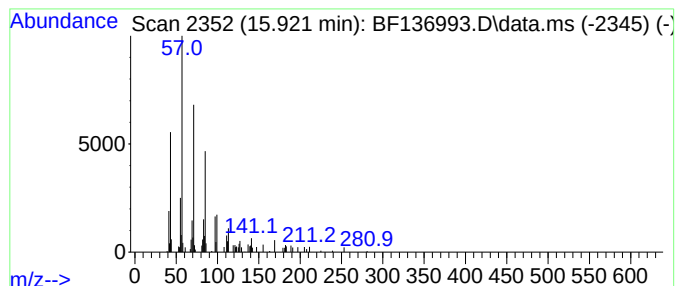
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octacosane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	2.74 ng	68219	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2			Tetratetracontane	619	C44H90	007098-22-8	90
3			Hexacosane	366	C26H54	000630-01-3	87
4			Octacosane	394	C28H58	000630-02-4	86
5			Octadecane	254	C18H38	000593-45-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010824\
Data File : BF136993.D
Acq On : 08 Jan 2024 12:41
Operator : CG\JU
Sample : PB158263BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158263BL

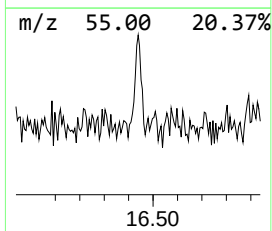
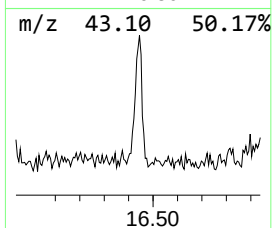
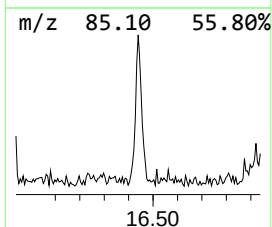
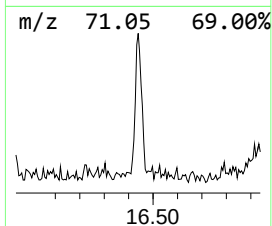
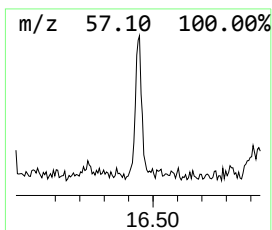
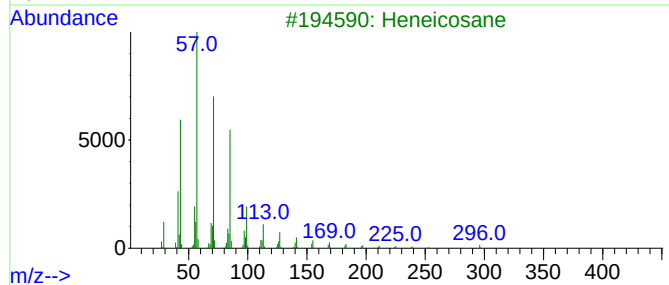
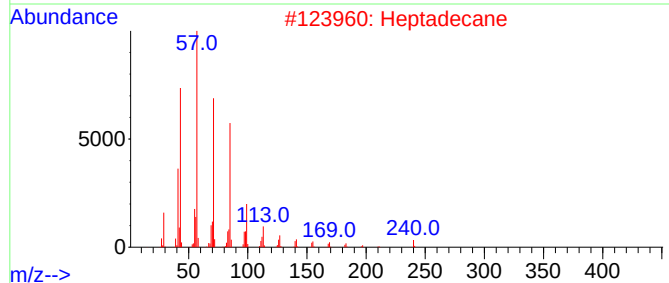
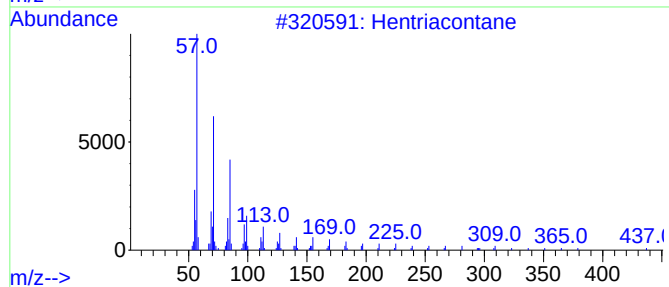
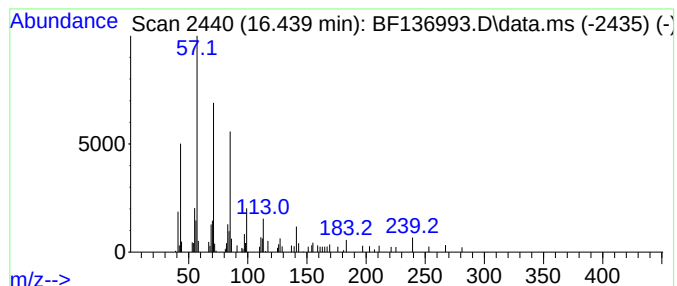
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Hentriacontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.439	2.60 ng	64794	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Heptadecane	240	C17H36	000629-78-7	87
3			Heneicosane	296	C21H44	000629-94-7	87
4			Octadecane	254	C18H38	000593-45-3	86
5			Octacosane	394	C28H58	000630-02-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010824\
Data File : BF136993.D
Acq On : 08 Jan 2024 12:41
Operator : CG\JU
Sample : PB158263BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158263BL

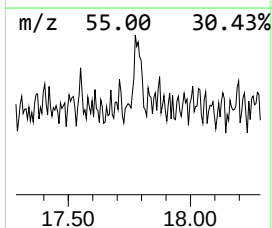
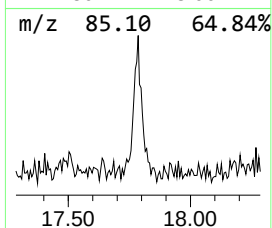
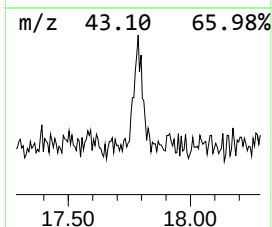
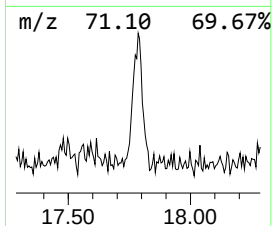
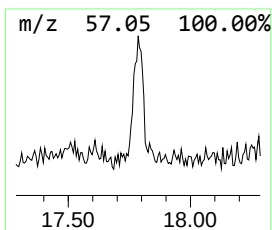
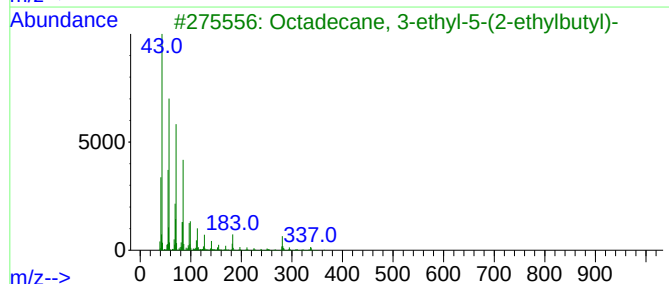
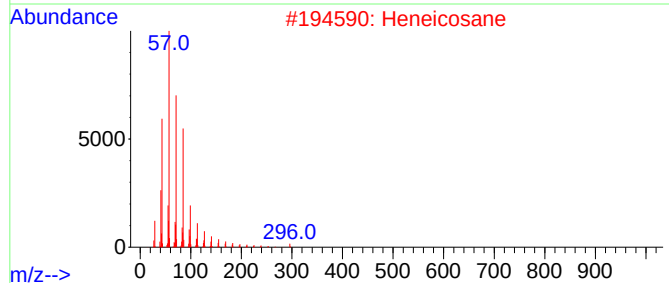
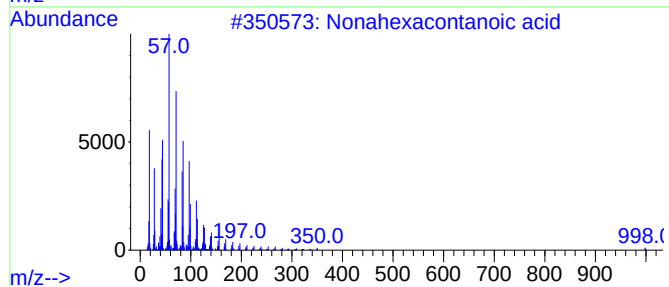
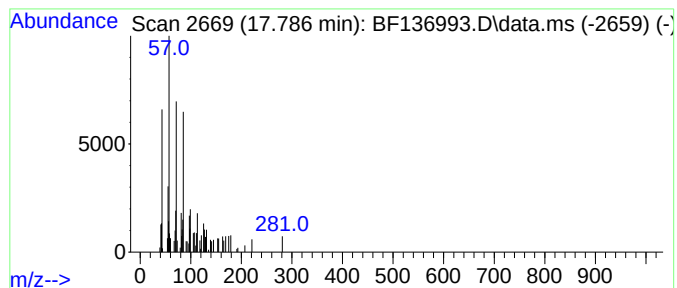
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Nonahexacontanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.786	2.33 ng	58176	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonahexacontanoic acid	999	C69H138O2	040710-32-5	72
2			Heneicosane	296	C21H44	000629-94-7	64
3			Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	64
4			2-Bromo dodecane	248	C12H25Br	013187-99-0	59
5			Hexadecane	226	C16H34	000544-76-3	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010824\
Data File : BF136993.D
Acq On : 08 Jan 2024 12:41
Operator : CG\JU
Sample : PB158263BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158263BL

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
2-Pentanone, 4-...	5.063	3.2	ng	74722	1	6.781	465550	20.0
Octacosane, 2-m...	15.921	2.7	ng	68219	6	15.457	498372	20.0
Hentriacontane	16.439	2.6	ng	64794	6	15.457	498372	20.0
Nonahexacontano...	17.786	2.3	ng	58176	6	15.457	498372	20.0