

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082923\
 Data File : BF134980.D
 Acq On : 29 Aug 2023 13:04
 Operator : CG\JU
 Sample : PB155117BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB155117BL

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-BF082223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134980.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.045	499	503	511	rVB	52125	73291	1.72%	0.277%
2	5.428	562	568	571	rBV	3460815	3458181	81.37%	13.051%
3	6.428	732	738	741	rBV	3220639	3442137	80.99%	12.991%
4	6.786	795	799	802	rBV	778391	679255	15.98%	2.564%
5	7.345	889	894	897	rBV	2113757	2286173	53.79%	8.628%
6	8.063	1011	1016	1020	rBV	1050264	915553	21.54%	3.455%
7	9.145	1194	1200	1203	rBV	4385869	4155668	97.78%	15.684%
8	9.822	1310	1315	1318	rBV	1280606	1046005	24.61%	3.948%
9	10.616	1445	1450	1453	rBV	2989283	2749140	64.69%	10.375%
10	11.310	1564	1568	1572	rBV	1233841	1072278	25.23%	4.047%
11	11.845	1654	1659	1673	rBV2	54335	99052	2.33%	0.374%
12	12.916	1836	1841	1844	rBV	4241562	4249888	100.00%	16.039%
13	13.910	1998	2010	2012	rBV5	49200	127482	3.00%	0.481%
14	13.962	2016	2019	2026	rVB	751524	744461	17.52%	2.810%
15	14.139	2044	2049	2056	rBV	71479	79057	1.86%	0.298%
16	14.445	2096	2101	2106	rBV	118720	138827	3.27%	0.524%
17	14.757	2149	2154	2159	rBV	122102	134556	3.17%	0.508%
18	15.098	2208	2212	2220	rVB	101965	127304	3.00%	0.480%
19	15.433	2265	2269	2274	rVB	511951	626981	14.75%	2.366%
20	15.486	2274	2278	2285	rVB	65690	94249	2.22%	0.356%
21	15.927	2349	2353	2358	rVB3	39532	62505	1.47%	0.236%
22	16.939	2515	2525	2537	rVB5	32218	134827	3.17%	0.509%

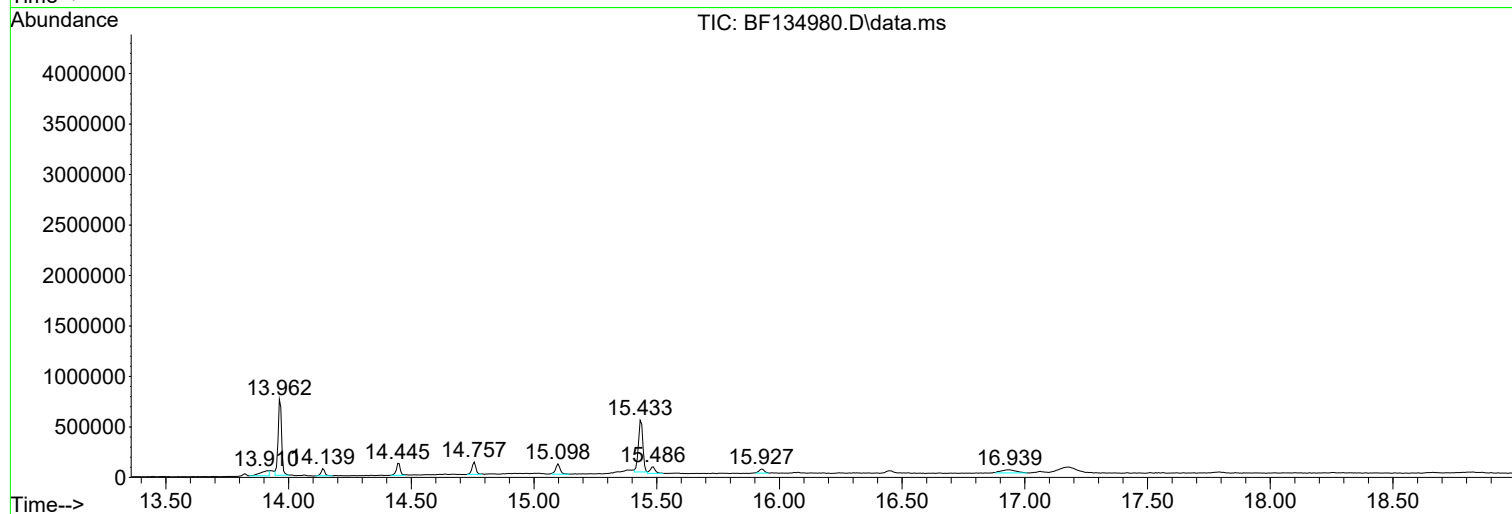
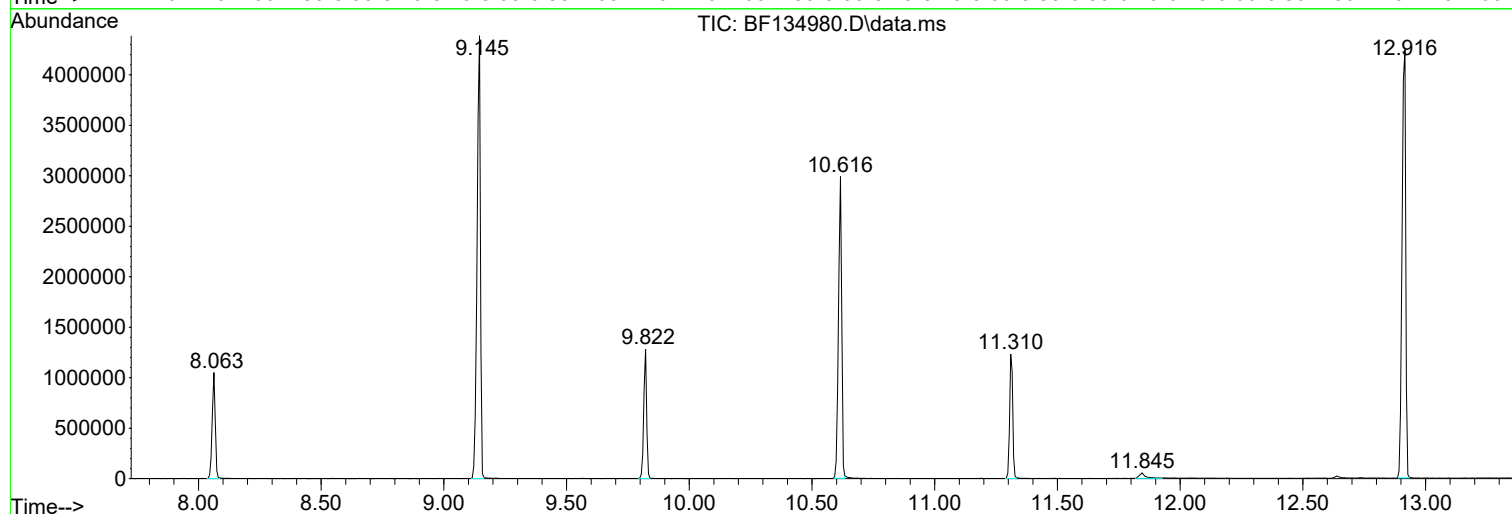
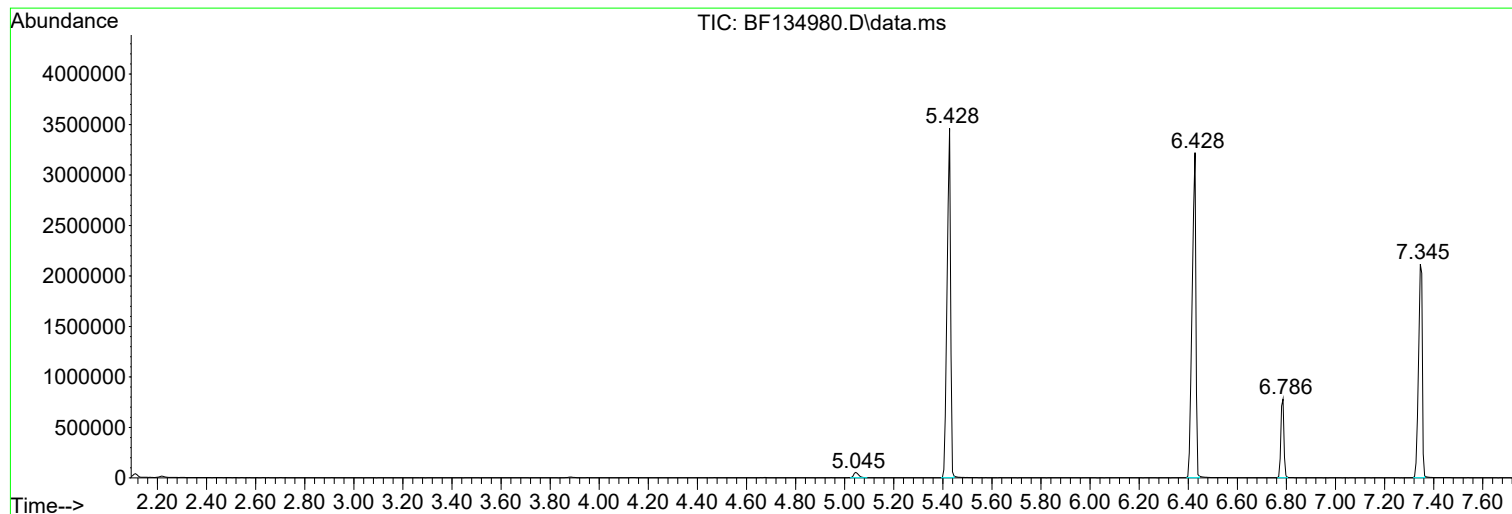
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF134980.D
Acq On : 29 Aug 2023 13:04
Operator : CG\JU
Sample : PB155117BL
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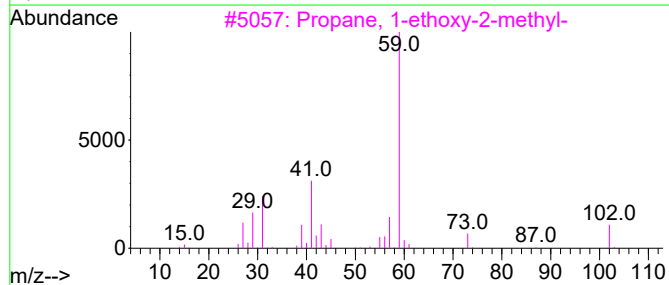
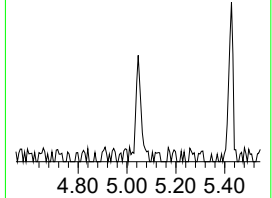
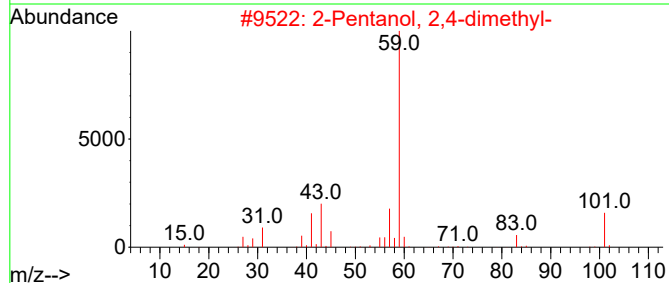
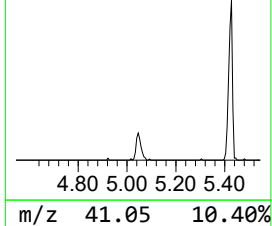
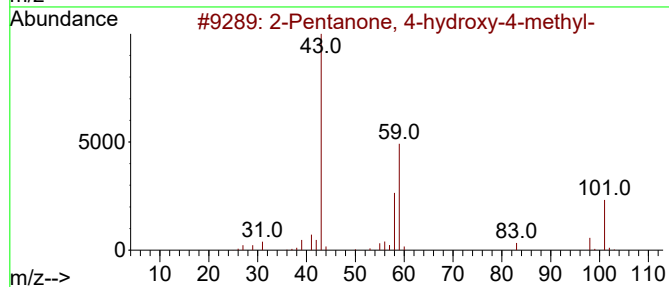
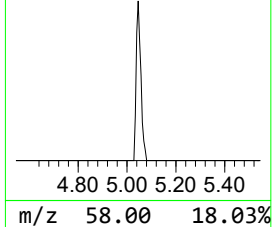
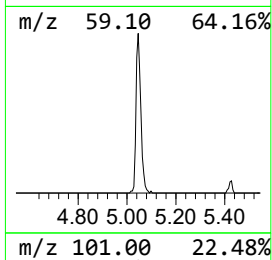
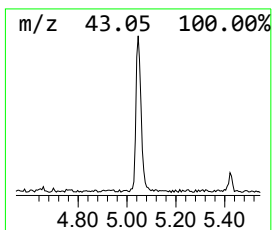
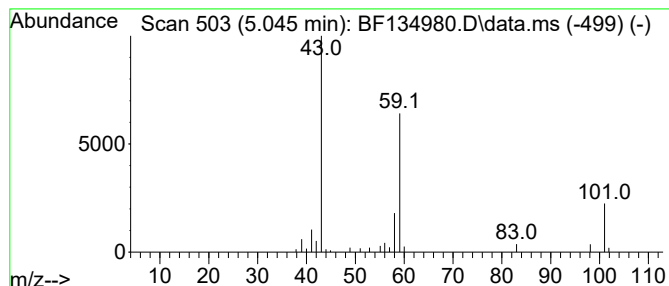
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.045	2.16 ng	73291	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	42
2	2-Pentanol, 2,4-dimethyl-		116	C7H16O	000625-06-9	40
3	Propane, 1-ethoxy-2-methyl-		102	C6H14O	000627-02-1	38
4	3-Hydroxy-3-methyl-2-butanone		102	C5H10O2	000115-22-0	12
5	(+) -4-Amino-4,5-dihydro-2(3H)-f...		101	C4H7NO2	016504-58-8	9



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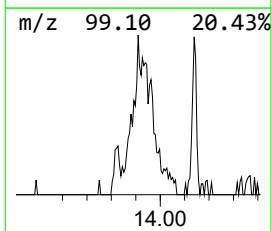
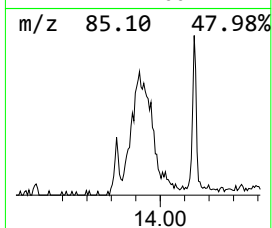
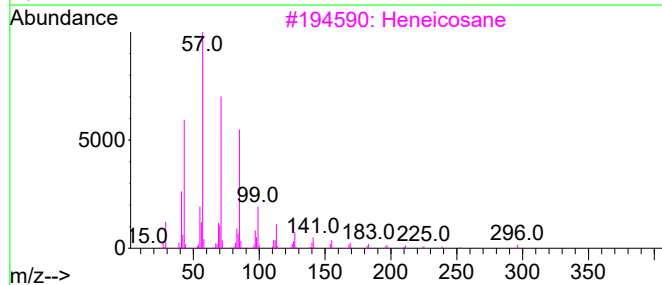
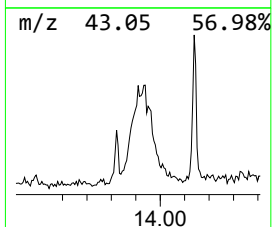
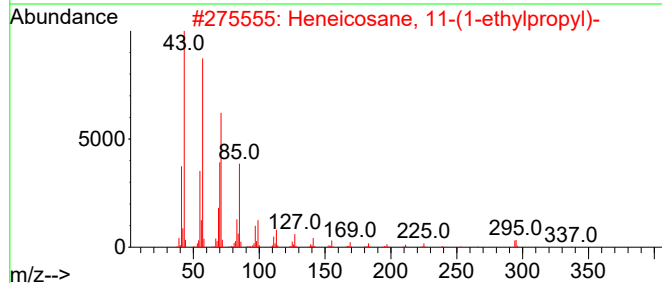
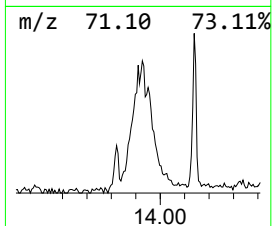
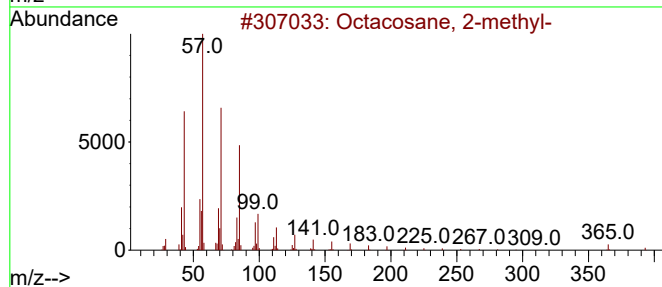
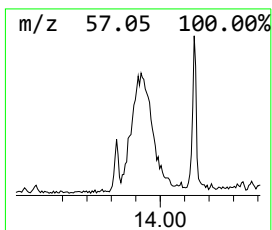
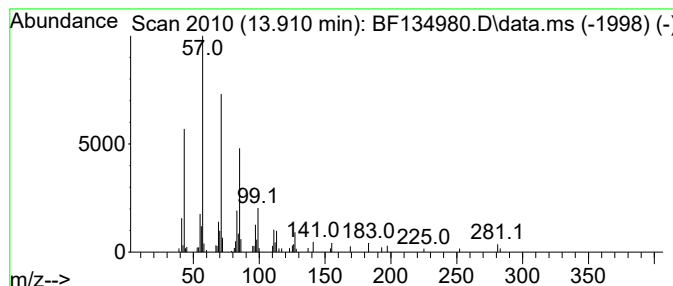
Instrument :
BNA_F
ClientSampleId :
PB155117BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.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 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.910	3.42 ng	127482	Chrysene-d12	13.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Tetratetracontane	619	C44H90	007098-22-8	87
5	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	80



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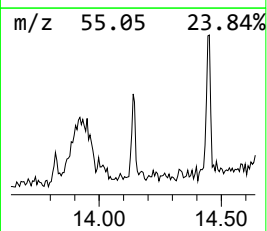
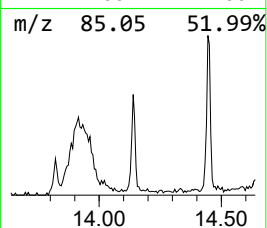
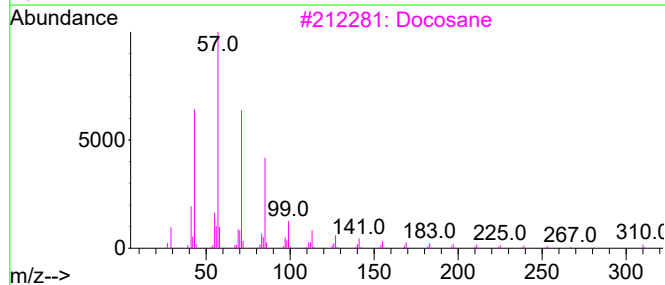
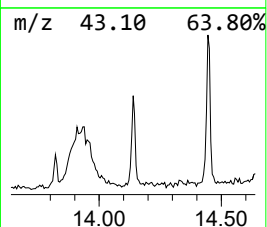
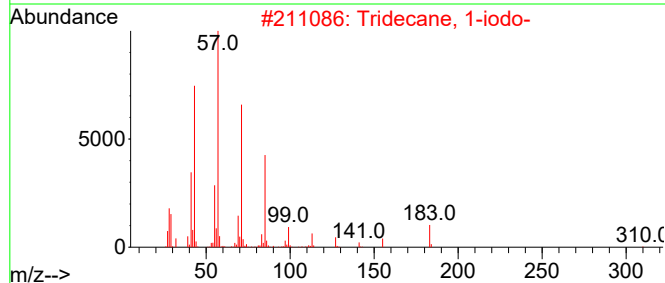
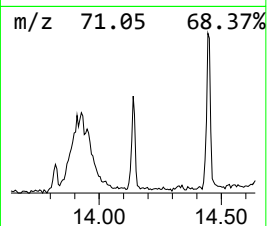
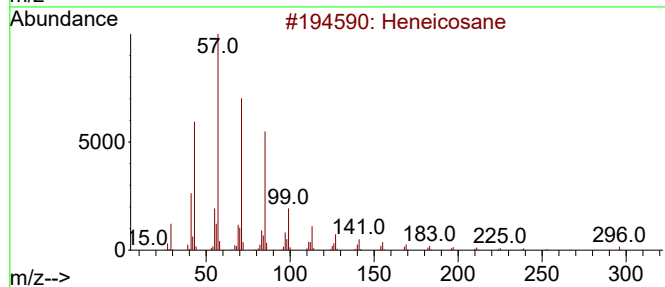
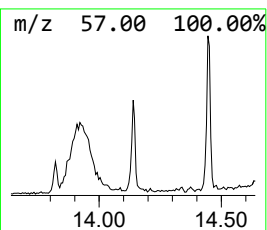
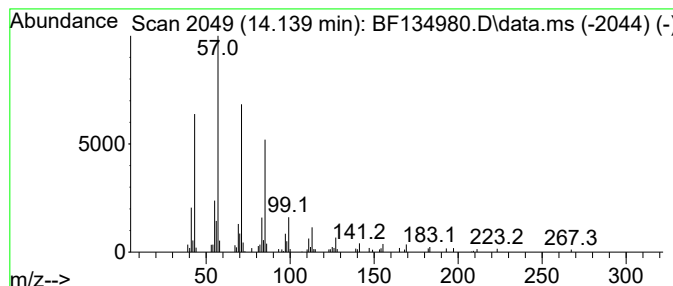
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.139	2.12 ng	79057	Chrysene-d12	13.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
3			Docosane	310	C22H46	000629-97-0	91
4			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	91
5			Eicosane	282	C20H42	000112-95-8	91



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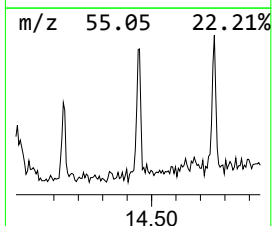
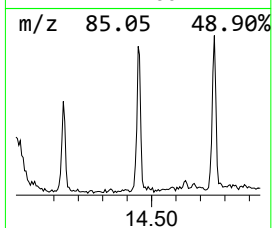
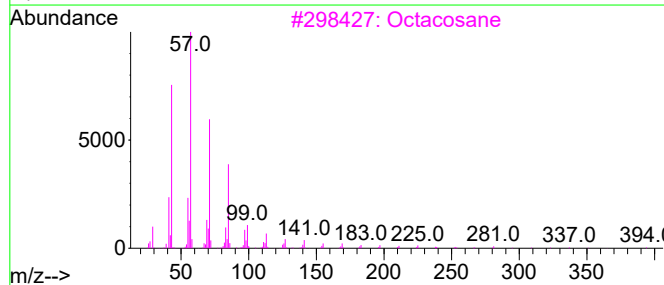
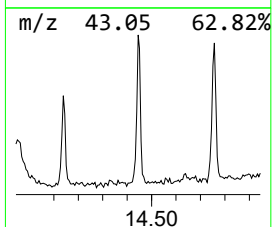
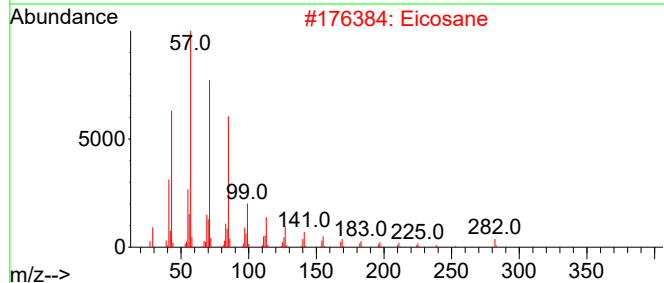
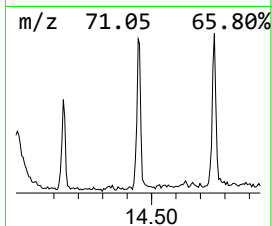
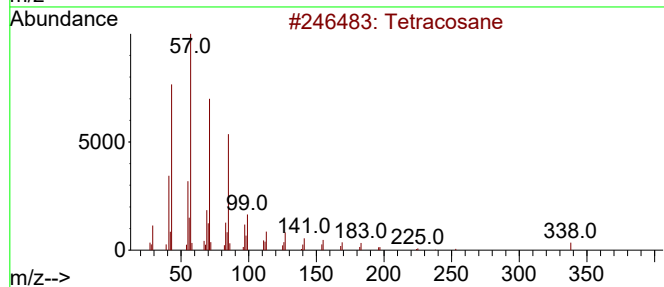
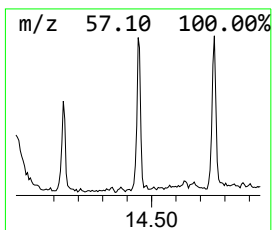
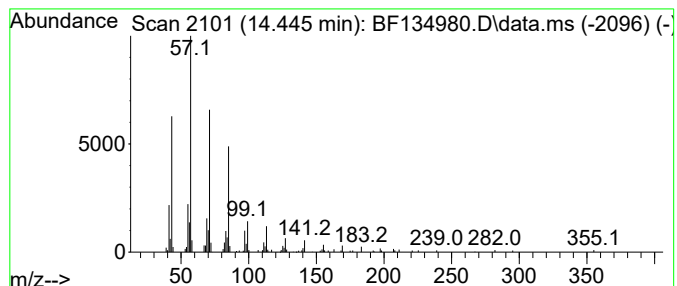
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.445	3.73 ng	138827	Chrysene-d12	13.963

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	91
2		Eicosane	282	C20H42	000112-95-8	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



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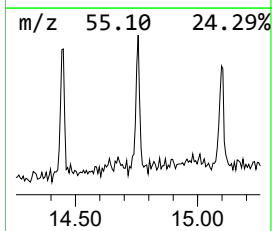
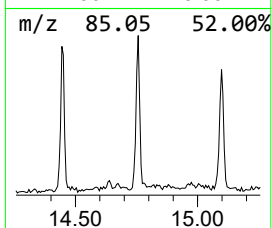
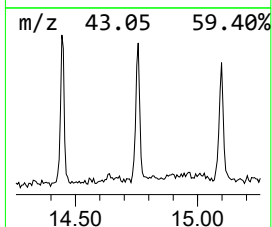
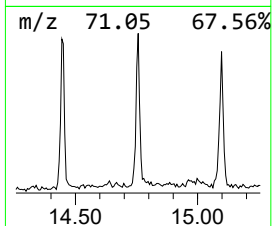
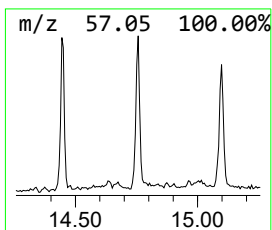
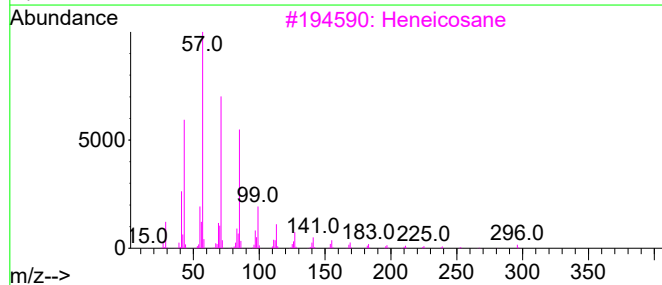
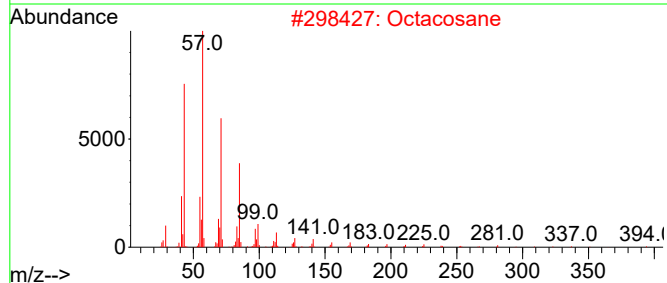
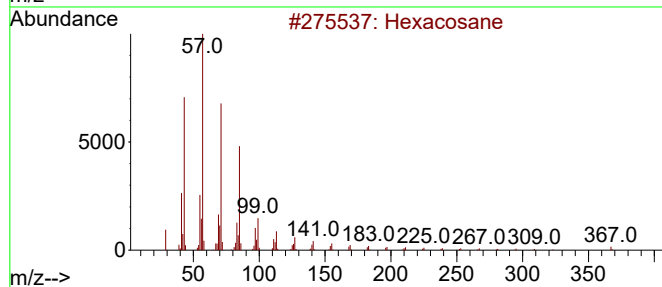
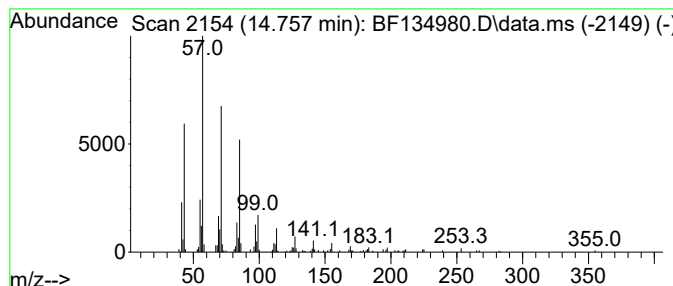
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Hexacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.757	4.29 ng	134556	Perylene-d12	15.433	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	93
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91



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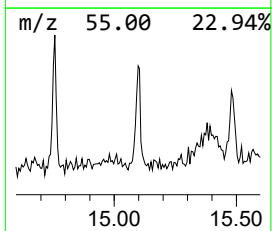
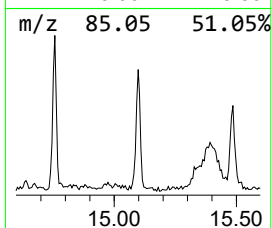
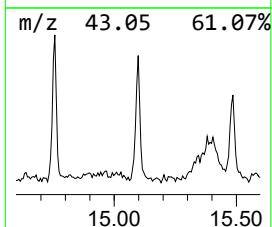
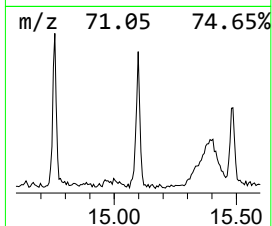
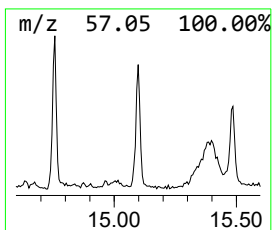
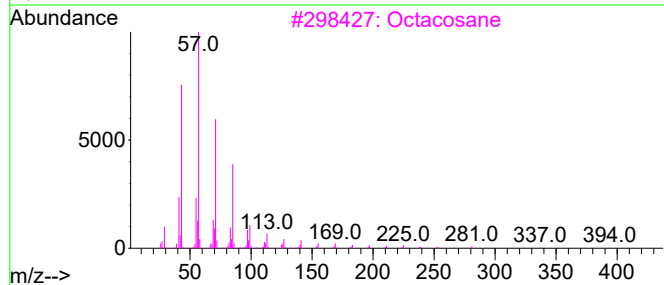
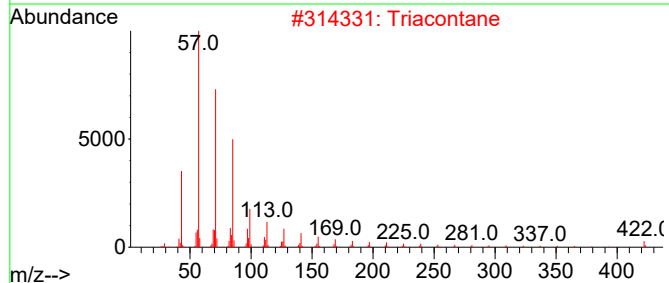
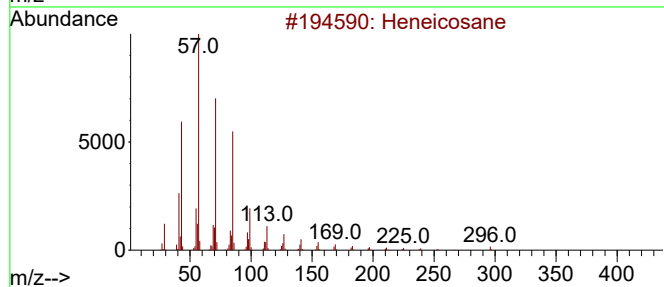
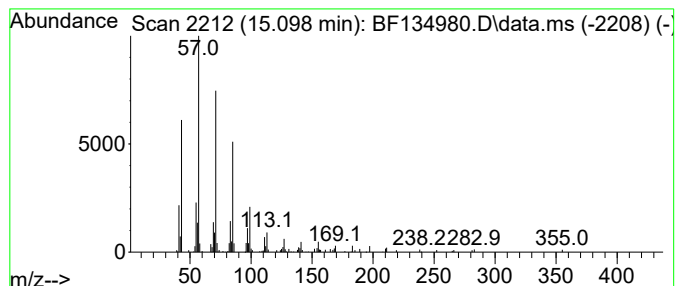
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triacontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.098	4.06 ng	127304	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Triacontane	422	C30H62	000638-68-6	87
3			Octacosane	394	C28H58	000630-02-4	87
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082923\
Data File : BF134980.D
Acq On : 29 Aug 2023 13:04
Operator : CG\JU
Sample : PB155117BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB155117BL

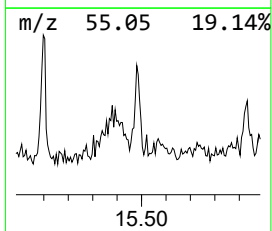
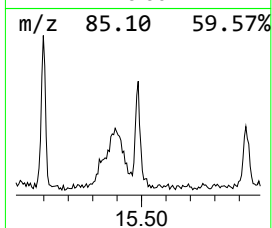
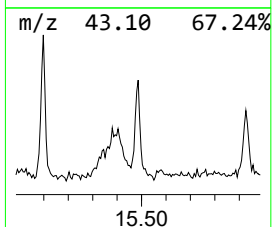
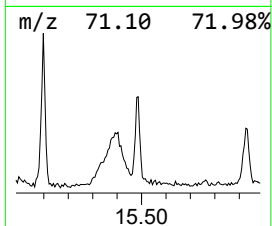
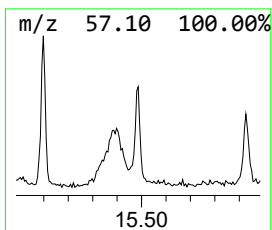
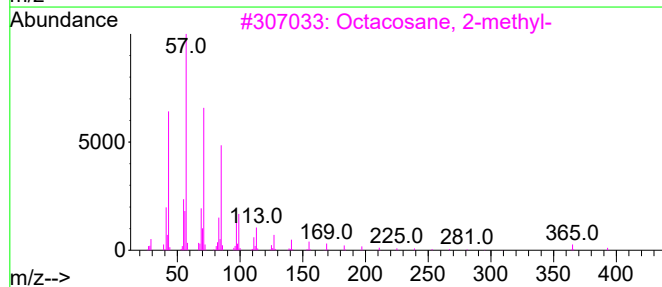
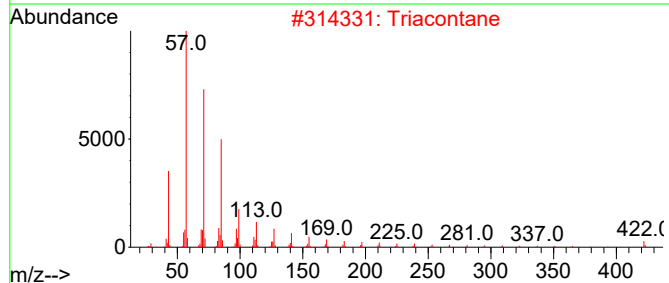
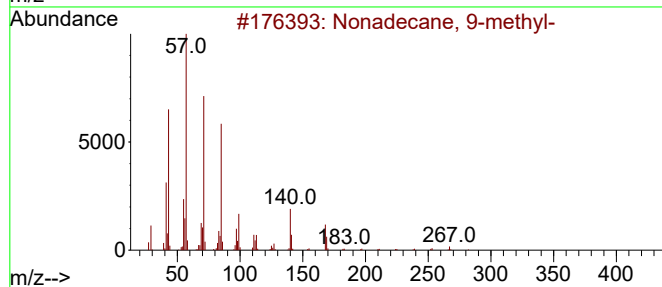
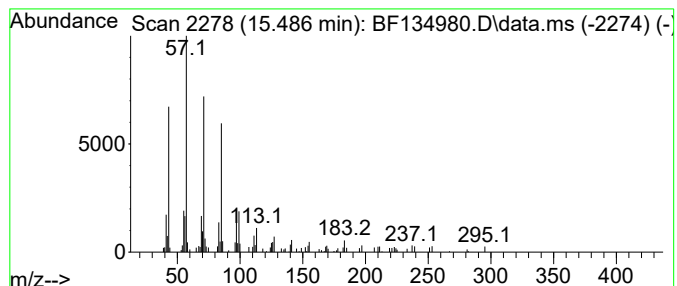
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane, 9-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.486	3.01 ng	94249	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2			Triacontane	422	C30H62	000638-68-6	90
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
4			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	89
5			Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082923\
Data File : BF134980.D
Acq On : 29 Aug 2023 13:04
Operator : CG\JU
Sample : PB155117BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

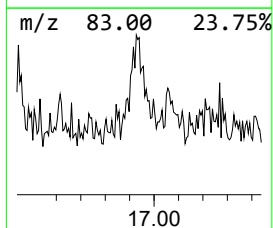
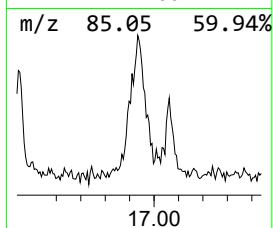
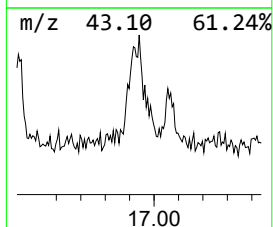
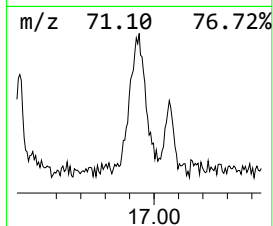
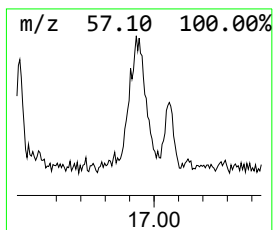
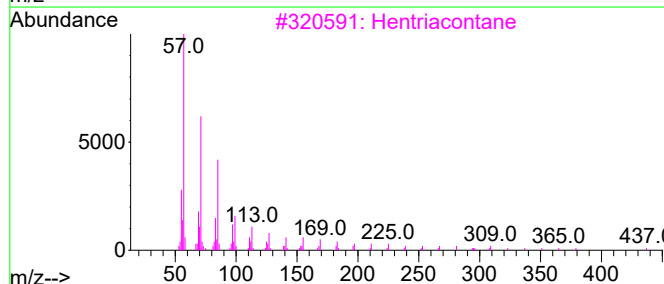
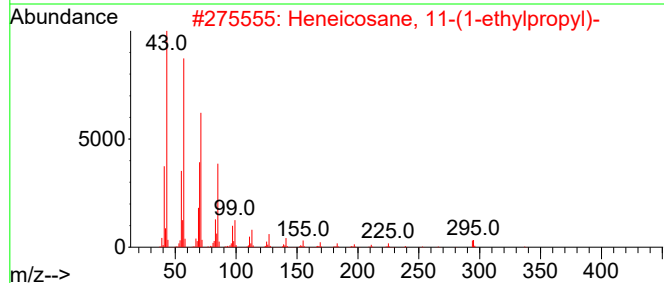
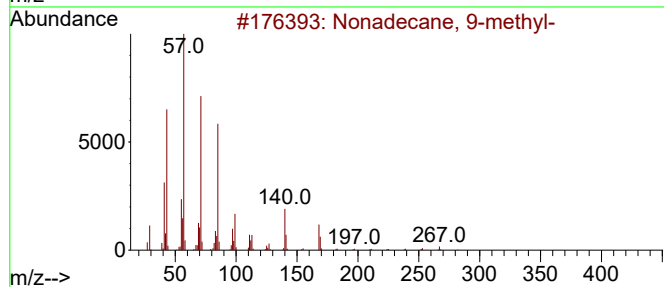
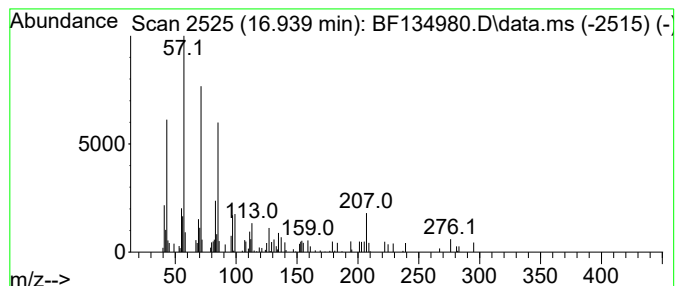
Instrument :
BNA_F
ClientSampleId :
PB155117BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane, 11-(1-ethylpro... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.939	4.30 ng	134827	Perylene-d12	15.433	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80
3	Hentriacontane	437	C31H64	000630-04-6	74
4	Pentacosane	352	C25H52	000629-99-2	74
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082923\
Data File : BF134980.D
Acq On : 29 Aug 2023 13:04
Operator : CG\JU
Sample : PB155117BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB155117BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF082223.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-...	5.045	2.2	ng	73291	1	6.786	679255	20.0
Octacosane, 2-m...	13.910	3.4	ng	127482	5	13.963	744461	20.0
Heneicosane	14.139	2.1	ng	79057	5	13.963	744461	20.0
Tetracosane	14.445	3.7	ng	138827	5	13.963	744461	20.0
Hexacosane	14.757	4.3	ng	134556	6	15.433	626981	20.0
triacontane	15.098	4.1	ng	127304	6	15.433	626981	20.0
Nonadecane, 9-m...	15.486	3.0	ng	94249	6	15.433	626981	20.0
Heneicosane, 11...	16.939	4.3	ng	134827	6	15.433	626981	20.0