LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139316.D
Acq On : 11 Sep 2024 10:50
Operator : RC/JU
Sample : PB163259BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163259BL

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-BF090424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139316.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.252	19	27	32	rVB	79604	132033	2.49%	0.384%
2	5.128	510	516	529	rVB	172318	326528	6.17%	0.950%
3	5.516	574	582	587	rBV	2891261	4398271	83.06%	12.800%
4	6.516	744	752	757	rBV	2813665	4553978	86.00%	13.254%
5	6.881	809	814	819	rBV	795285	992720	18.75%	2.889%
6	7.445	903	910	915	rBV	2083309	2996641	56.59%	8.721%
7	8.163	1026	1032	1037	rBV	1001526	1296395	24.48%	3.773%
8	9.239	1208	1215	1221	rBV	3714724	5295300	100.00%	15.411%
9	9.916	1324	1330	1336	rBV	1135102	1493364	28.20%	4.346%
10	10.710	1458	1465	1470	rBV	2424940	3269343	61.74%	9.515%
11	11.404	1578	1583	1588	rBV	1270411	1603398	30.28%	4.666%
12	12.810	1818	1822	1828	rVB	56979	68000	1.28%	0.198%
13	12.998	1847	1854	1859	rBV	3628047	5132920	96.93%	14.938%
14	14.039	2026	2031	2038	rVB	802251	1041050	19.66%	3.030%
15	14.821	2159	2164	2172	rVB	50004	68009	1.28%	0.198%
16	15.163	2217	2222	2230	rVB	62400	90033	1.70%	0.262%
17	15.515	2275	2282	2286	rBV	509197	793623	14.99%	2.310%
18	15.551	2286	2288	2297	rVB	88227	110355	2.08%	0.321%
19	15.992	2357	2363	2373	rBV	80895	143081	2.70%	0.416%
20	16.510	2444	2451	2460	rBV	80818	158330	2.99%	0.461%
21	17.115	2545	2554	2568	rBV2	72529	190056	3.59%	0.553%
22	17.827	2667	2675	2687	rBV	45213	118384	2.24%	0.345%
23	18.680	2811	2820	2832	rBV3	28187	88557	1.67%	0.258%

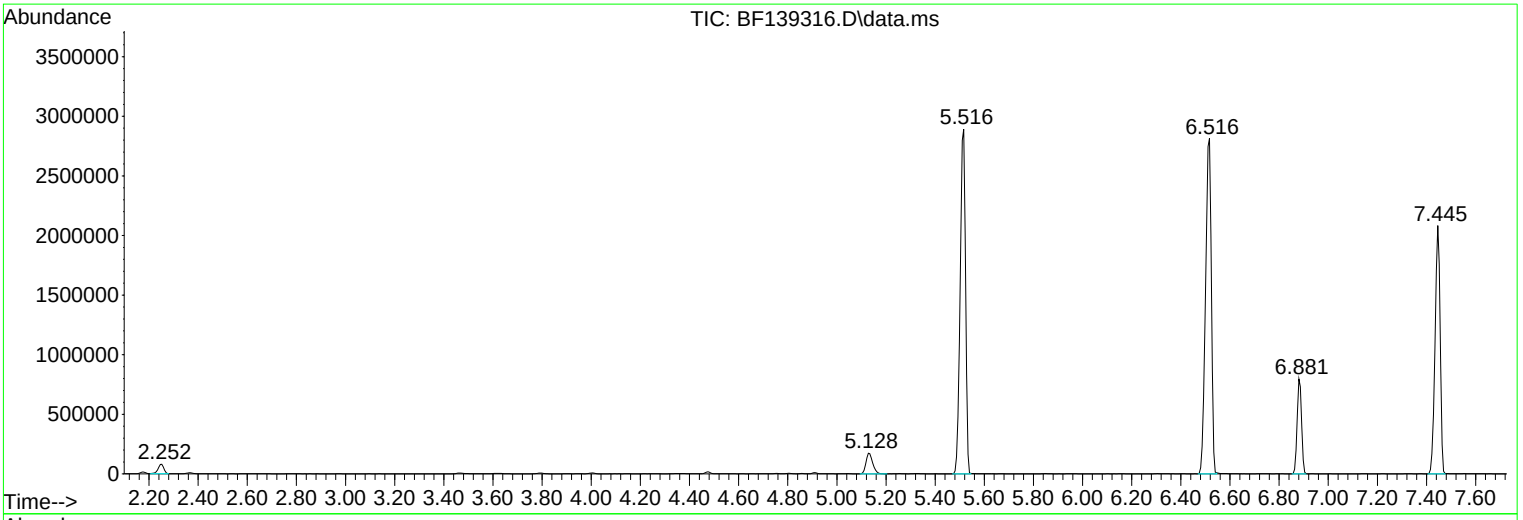
Sum of corrected areas: 34360369

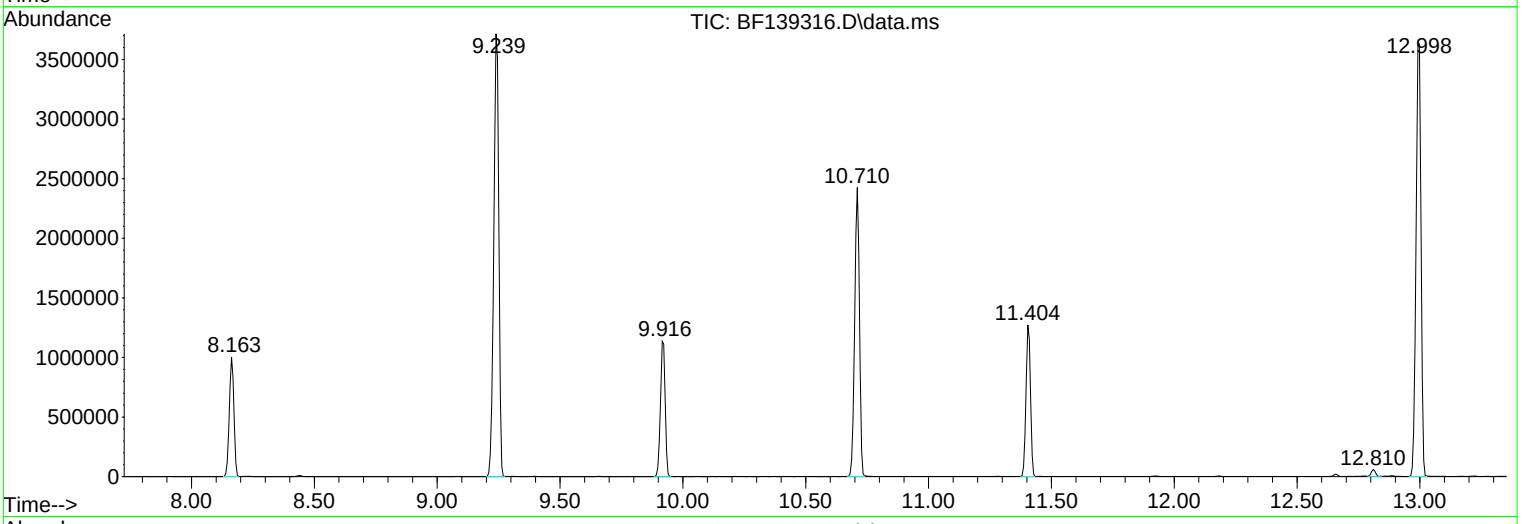
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139316.D
Acq On : 11 Sep 2024 10:50
Operator : RC/JU
Sample : PB163259BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

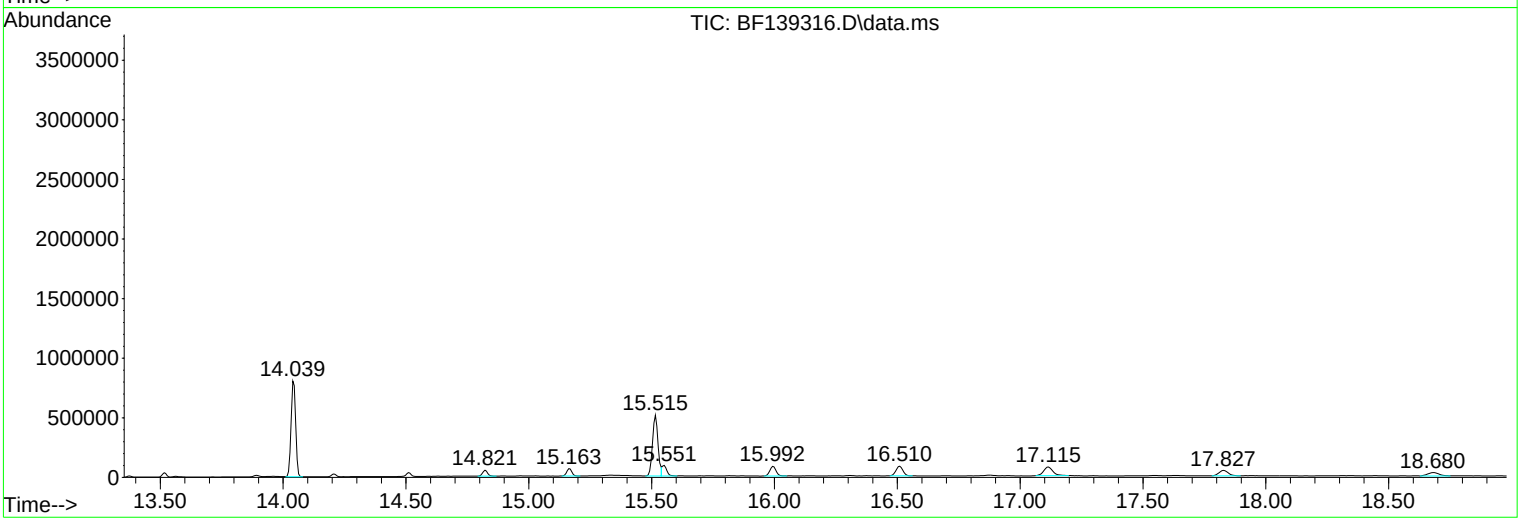
Instrument :
BNA_F
ClientSampleId :
PB163259BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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\BF091124\
Data File : BF139316.D
Acq On : 11 Sep 2024 10:50
Operator : RC/JU
Sample : PB163259BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163259BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

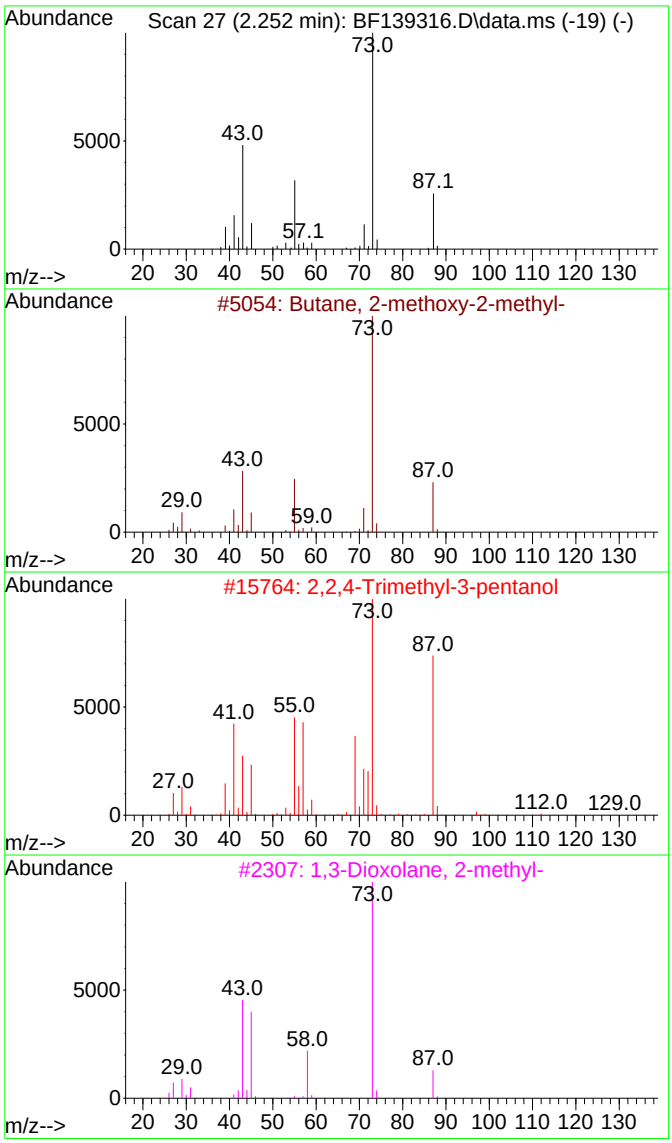
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

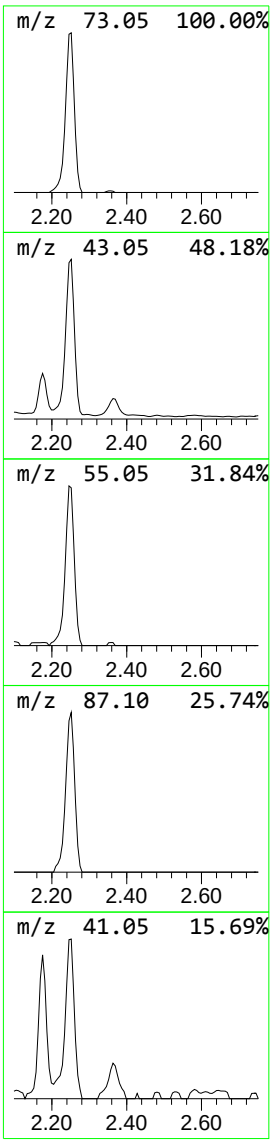
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.252	2.66 ng	132033	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139316.D
Acq On : 11 Sep 2024 10:50
Operator : RC/JU
Sample : PB163259BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163259BL

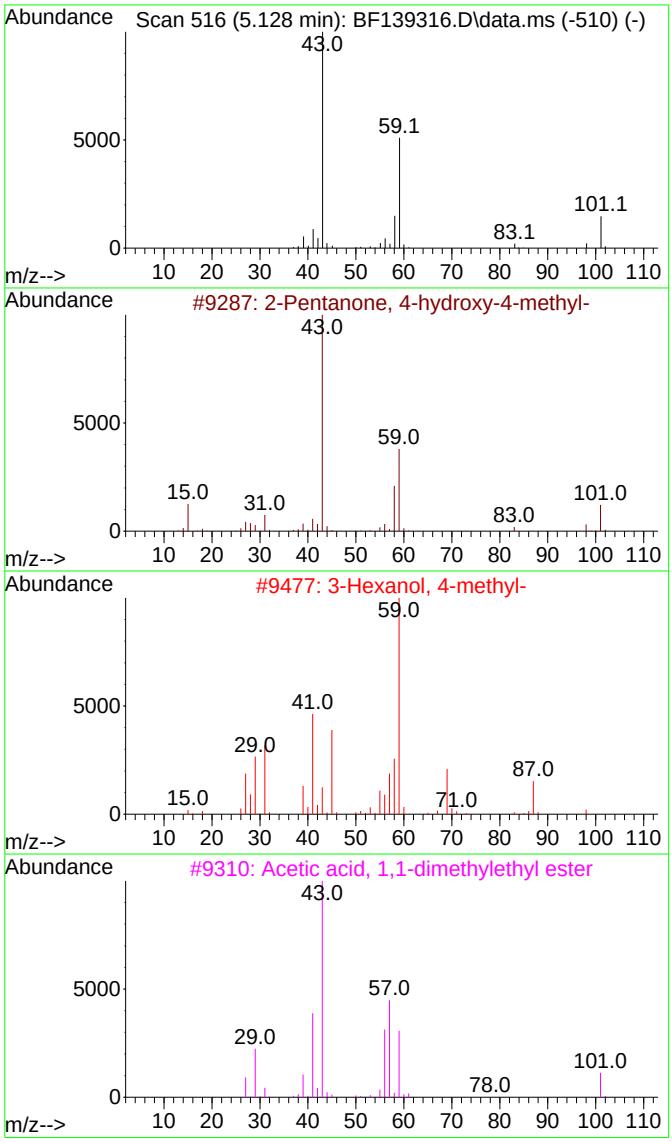
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

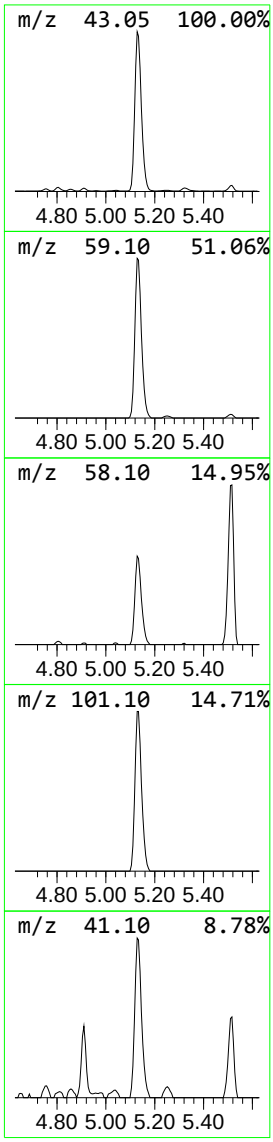
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	6.58 ng	326528	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139316.D
Acq On : 11 Sep 2024 10:50
Operator : RC/JU
Sample : PB163259BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163259BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

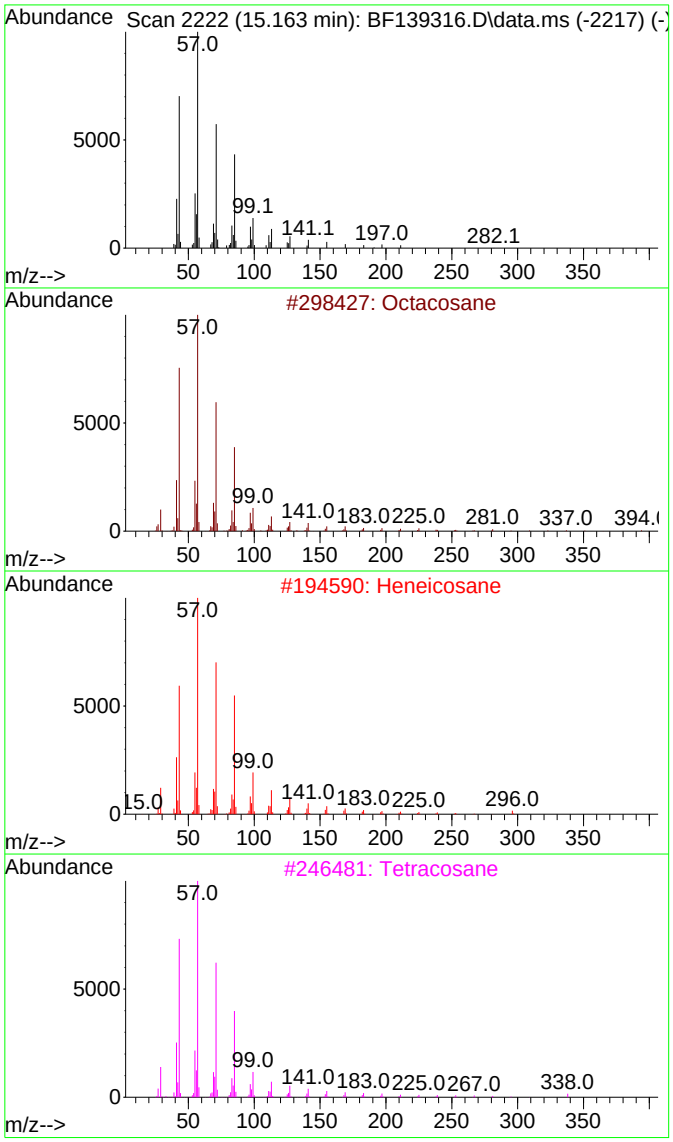
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

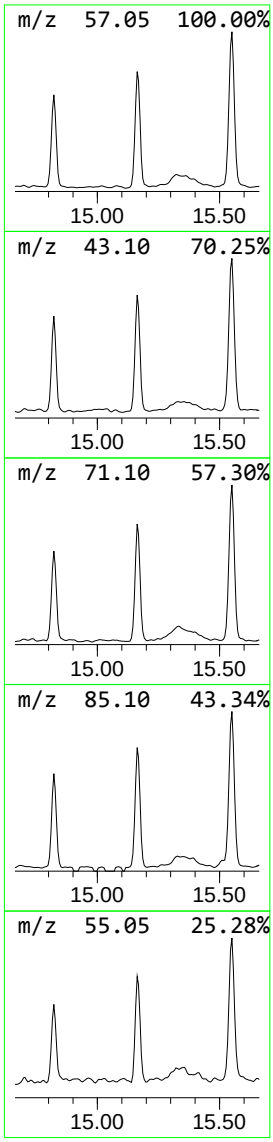
****

Peak Number 3 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	2.27 ng	90033	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Octadecane	254	C18H38	000593-45-3	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139316.D
Acq On : 11 Sep 2024 10:50
Operator : RC/JU
Sample : PB163259BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163259BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

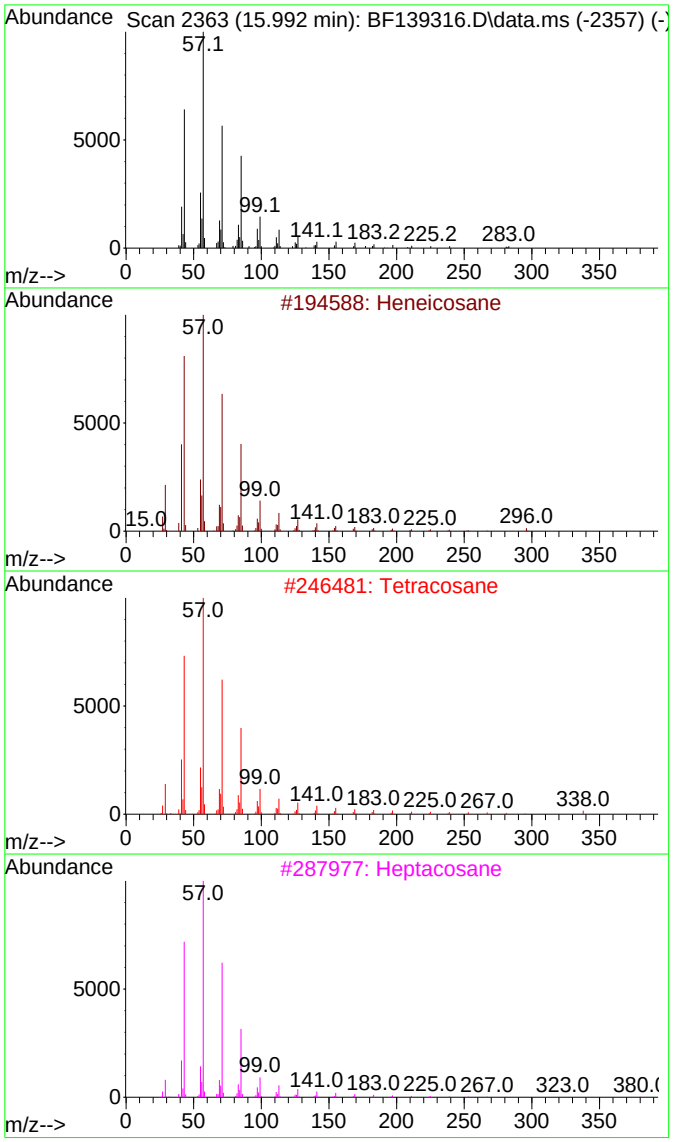
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

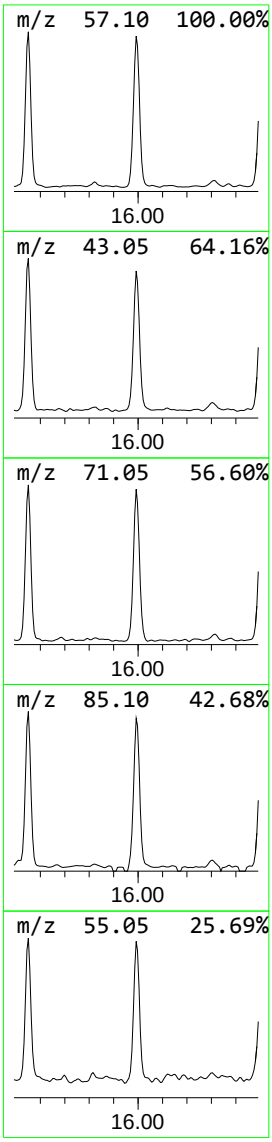
****

Peak Number 4 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.992	3.61 ng	143081	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Docosane	310	C22H46	000629-97-0	91
5	Hexacosane	366	C26H54	000630-01-3	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139316.D
Acq On : 11 Sep 2024 10:50
Operator : RC/JU
Sample : PB163259BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163259BL

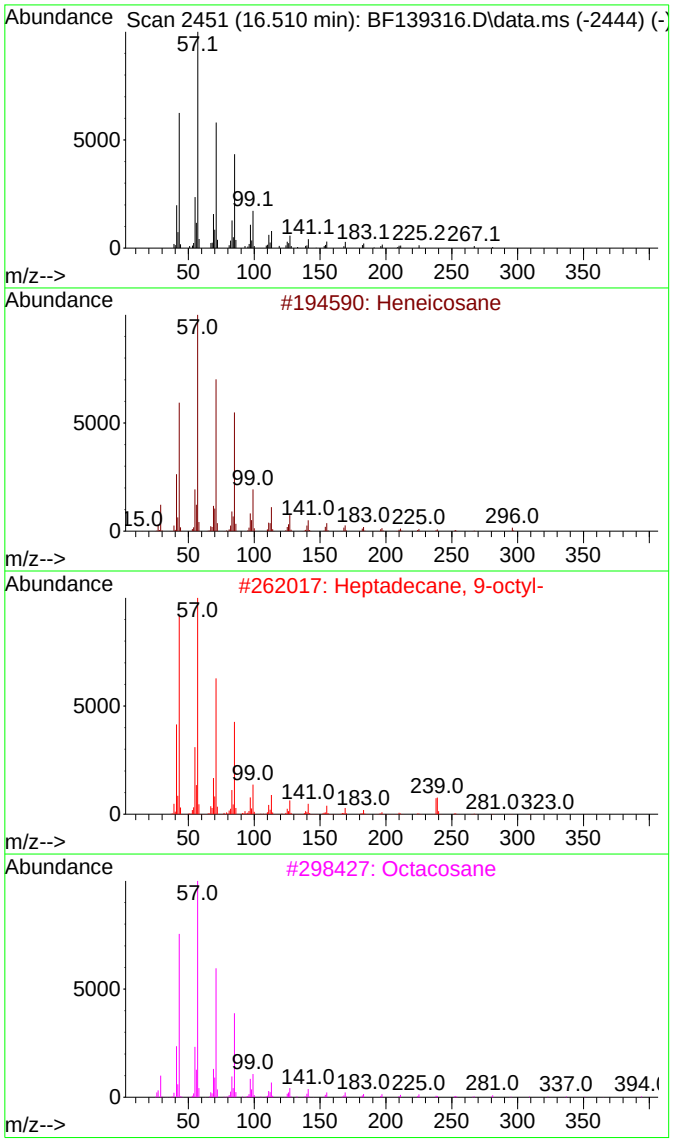
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

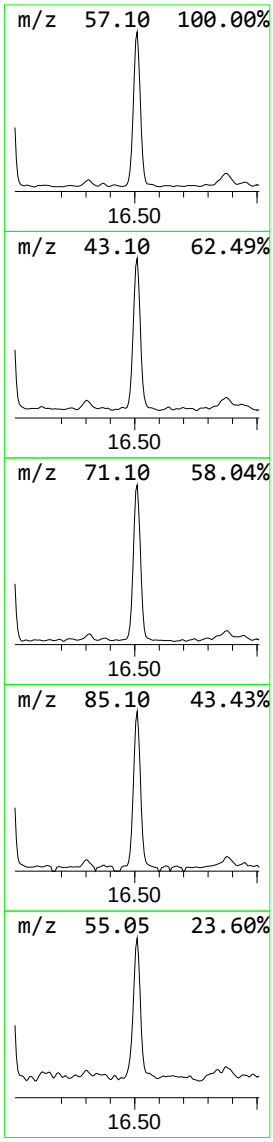
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Heptadecane, 9-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.509	3.99 ng	158330	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Hexacosane	366	C26H54	000630-01-3	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139316.D
Acq On : 11 Sep 2024 10:50
Operator : RC/JU
Sample : PB163259BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163259BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

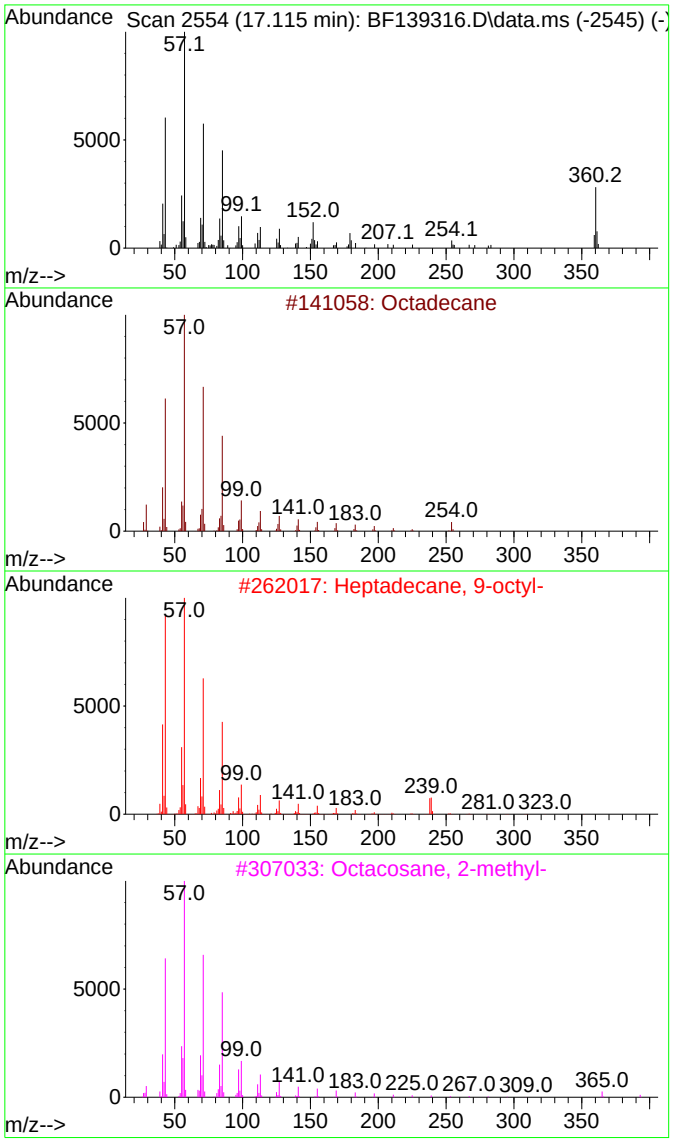
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

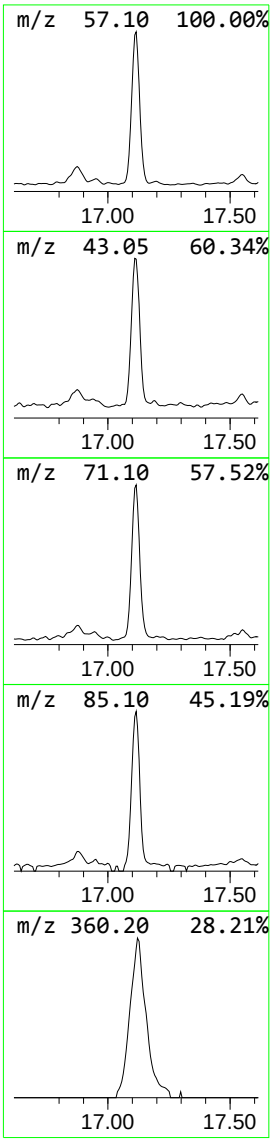
****

Peak Number 6 Octadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.115	4.79 ng	190056	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	98
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	64
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	64
4	Tetratetracontane	619	C44H90	007098-22-8	64
5	Hexacosane	366	C26H54	000630-01-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139316.D
Acq On : 11 Sep 2024 10:50
Operator : RC/JU
Sample : PB163259BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163259BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

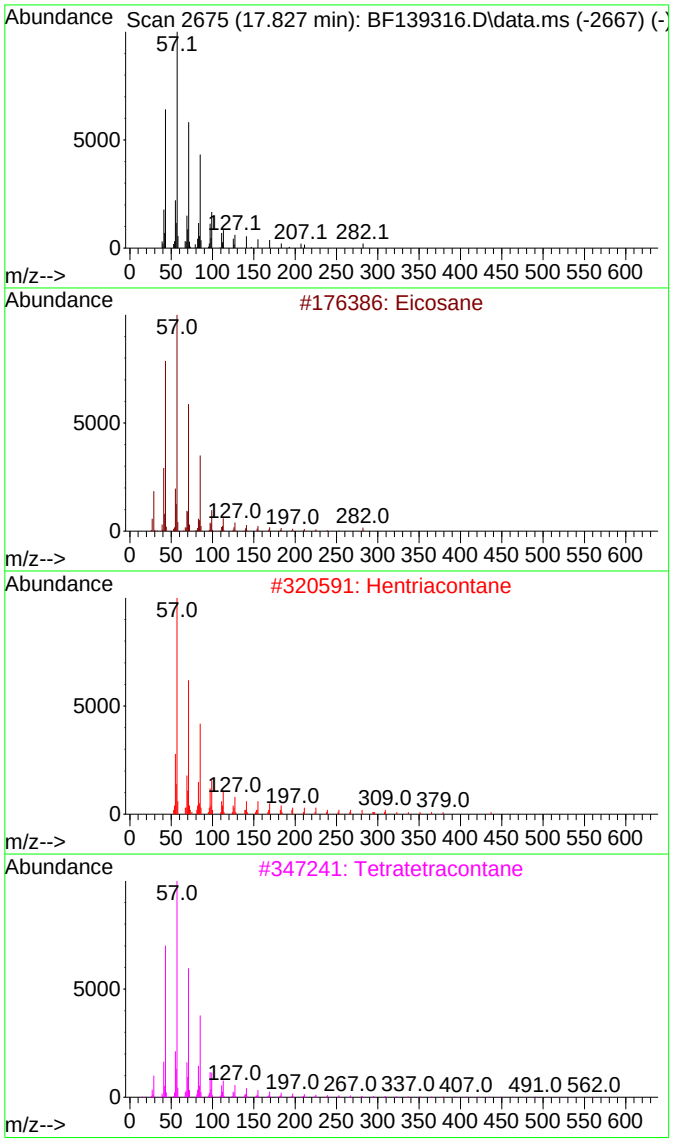
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

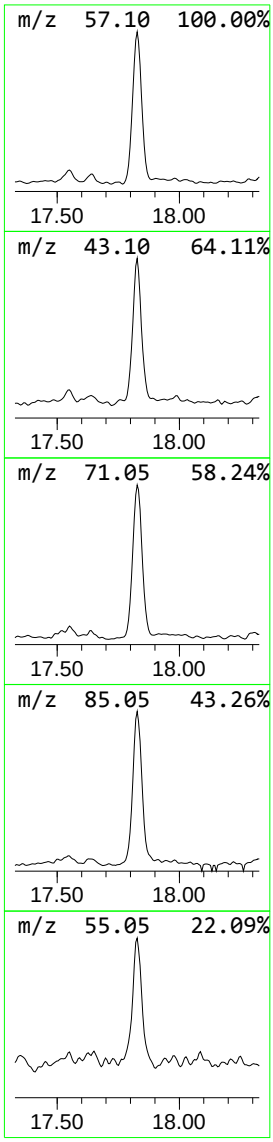
****

Peak Number 7 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.827	2.98 ng	118384	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heneicosane	296	C21H44	000629-94-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139316.D
Acq On : 11 Sep 2024 10:50
Operator : RC/JU
Sample : PB163259BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163259BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

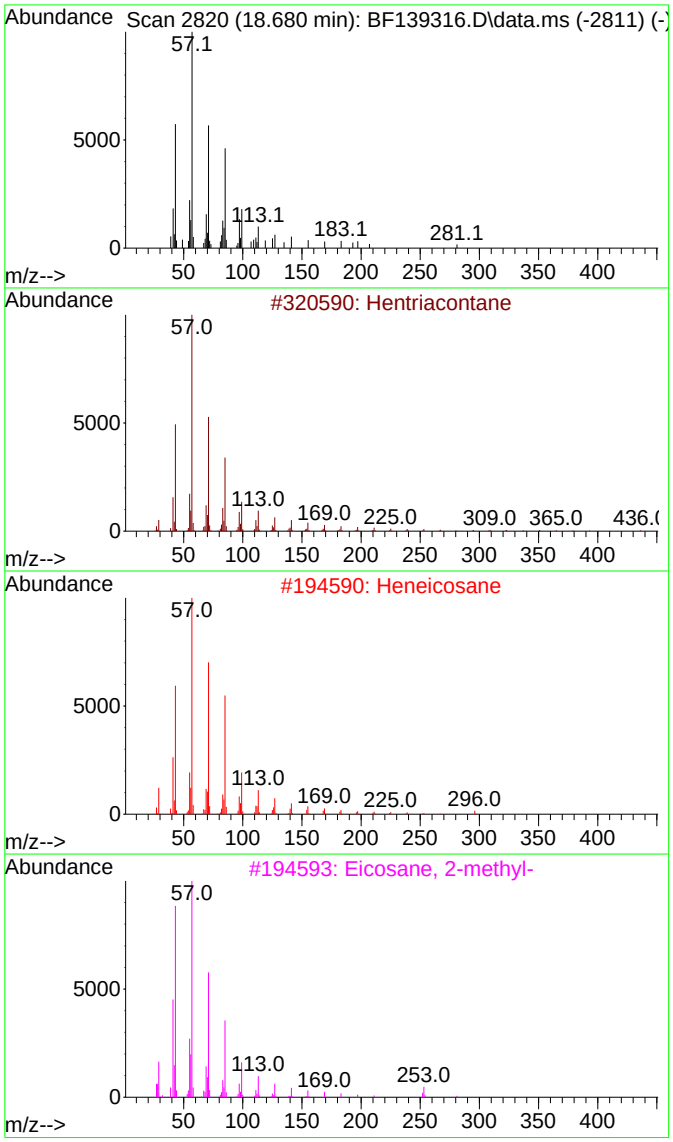
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

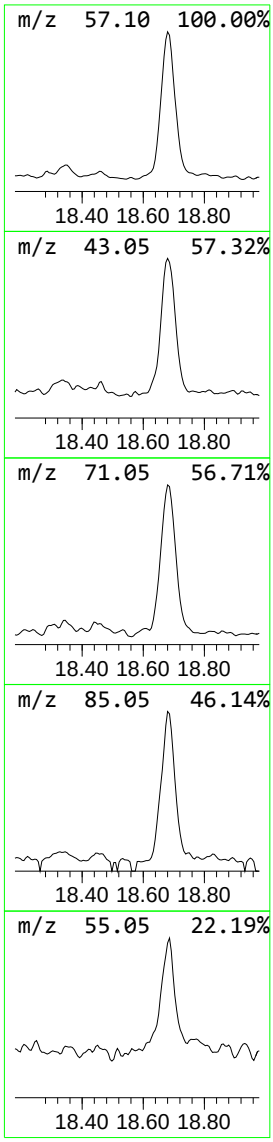
****

Peak Number 8 Hentriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.680	2.23 ng	88557	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Eicosane, 2-methyl-	296	C21H44	001560-84-5	90
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091124\
Data File : BF139316.D
Acq On : 11 Sep 2024 10:50
Operator : RC/JU
Sample : PB163259BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163259BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.252	2.7	ng	132033	1	6.881	992720	20.0
2-Pentanone, 4-...	5.128	6.6	ng	326528	1	6.881	992720	20.0
Octacosane	15.163	2.3	ng	90033	6	15.515	793623	20.0
Heneicosane	15.992	3.6	ng	143081	6	15.515	793623	20.0
Heptadecane, 9-...	16.509	4.0	ng	158330	6	15.515	793623	20.0
Octadecane	17.115	4.8	ng	190056	6	15.515	793623	20.0
Eicosane	17.827	3.0	ng	118384	6	15.515	793623	20.0
Hentriacontane	18.680	2.2	ng	88557	6	15.515	793623	20.0