LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131126.D
Acq On : 10 Nov 2022 16:51
Operator : CG\JU
Sample : PB148948BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148948BL

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-BF110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131126.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	15	25	33	rVB	117227	164774	5.71%	0.932%
2	2.340	39	43	51	rVB	44517	59215	2.05%	0.335%
3	5.128	512	517	529	rBV	260977	349996	12.14%	1.979%
4	5.516	578	583	586	rBV	2257663	2197047	76.19%	12.422%
5	6.516	748	753	756	rBV	1907997	2179779	75.59%	12.325%
6	6.887	812	816	820	rBV	589174	466803	16.19%	2.639%
7	7.457	907	913	916	rBV	1373656	1489529	51.66%	8.422%
8	8.175	1030	1035	1038	rBV	592979	586412	20.34%	3.316%
9	9.251	1212	1218	1221	rBV	2931780	2623954	91.00%	14.836%
10	9.934	1329	1334	1337	rBV	768850	664275	23.04%	3.756%
11	10.728	1462	1469	1472	rBV	1955561	1693296	58.72%	9.574%
12	11.428	1584	1588	1591	rBV	829846	677621	23.50%	3.831%
13	13.022	1854	1859	1862	rBV	3058738	2883567	100.00%	16.304%
14	14.074	2034	2038	2042	rBV	702696	632884	21.95%	3.578%
15	14.169	2049	2054	2061	rBV	36746	42051	1.46%	0.238%
16	14.845	2164	2169	2173	rBV2	30126	32382	1.12%	0.183%
17	15.192	2224	2228	2232	rBV	35712	40146	1.39%	0.227%
18	15.574	2287	2293	2305	rBV	392624	521608	18.09%	2.949%
19	16.033	2365	2371	2378	rBV	47812	73512	2.55%	0.416%
20	16.551	2453	2459	2466	rBV	53456	94750	3.29%	0.536%
21	17.168	2557	2564	2571	rBV3	31164	68143	2.36%	0.385%
22	17.898	2681	2688	2695	rVB2	30056	66752	2.31%	0.377%
23	18.756	2825	2834	2845	rBV5	22792	77600	2.69%	0.439%

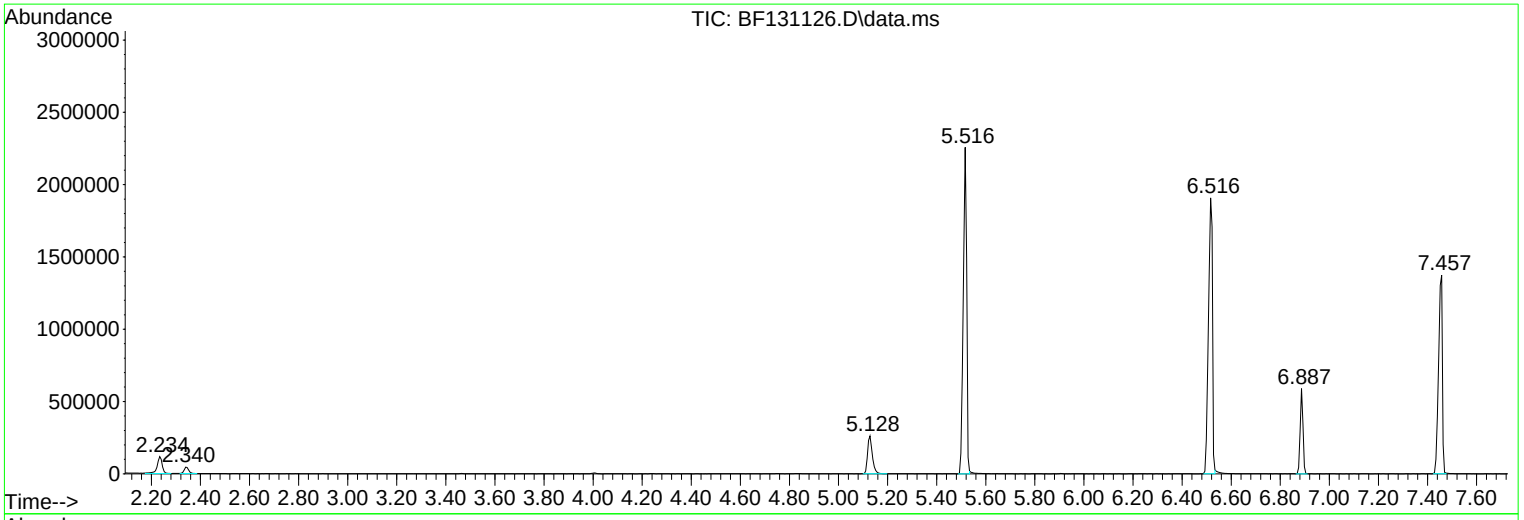
Sum of corrected areas: 17686096

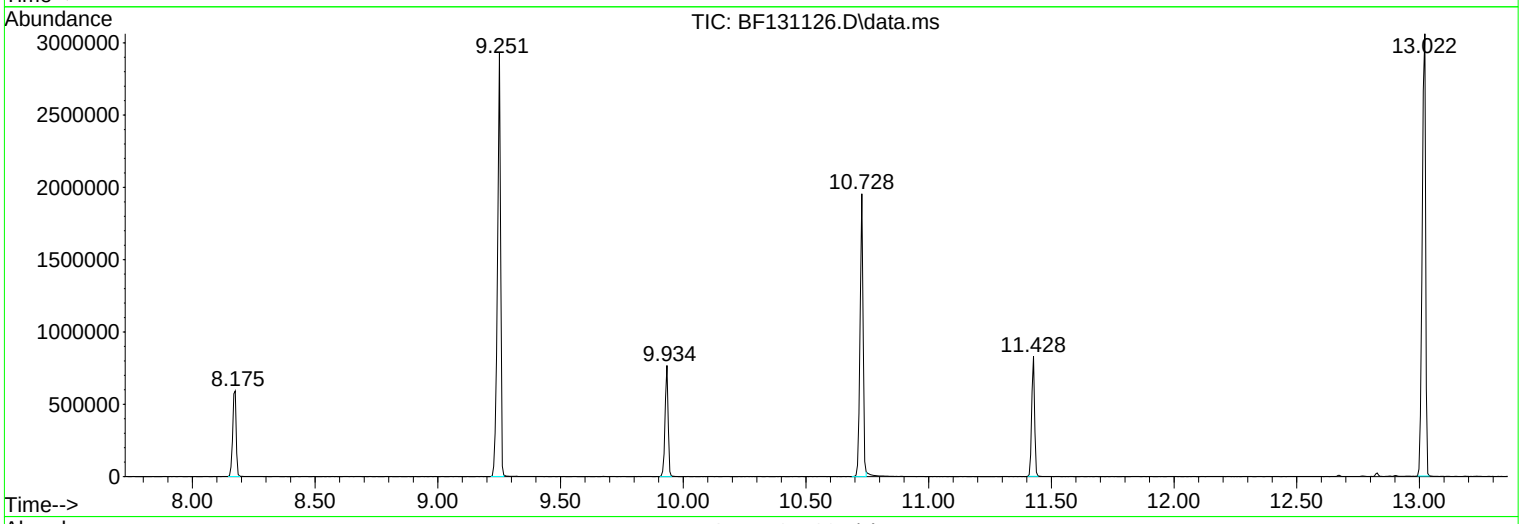
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131126.D
Acq On : 10 Nov 2022 16:51
Operator : CG\JU
Sample : PB148948BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

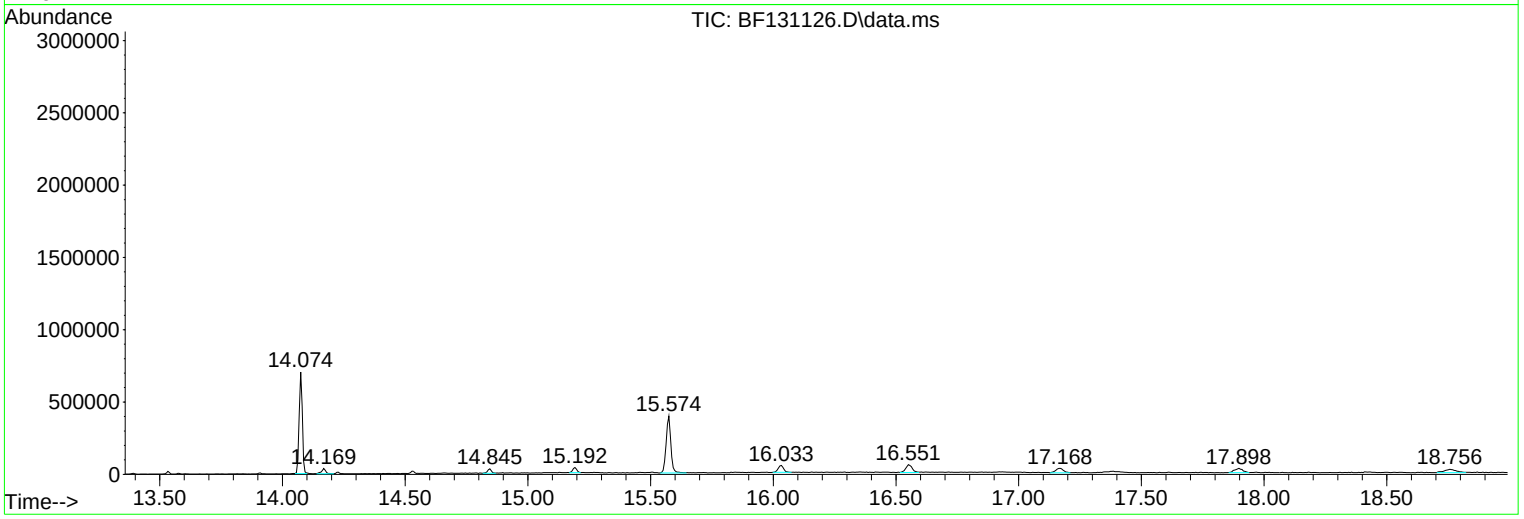
Instrument :
BNA_F
ClientSampleId :
PB148948BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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\BF111022\
Data File : BF131126.D
Acq On : 10 Nov 2022 16:51
Operator : CG\JU
Sample : PB148948BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148948BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

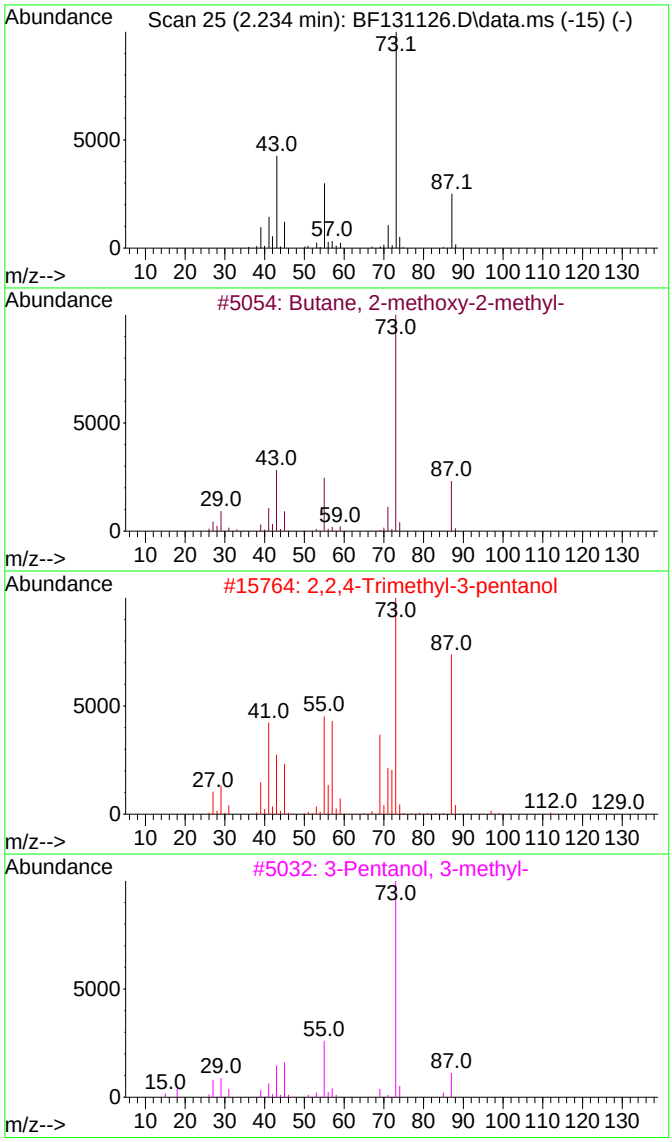
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

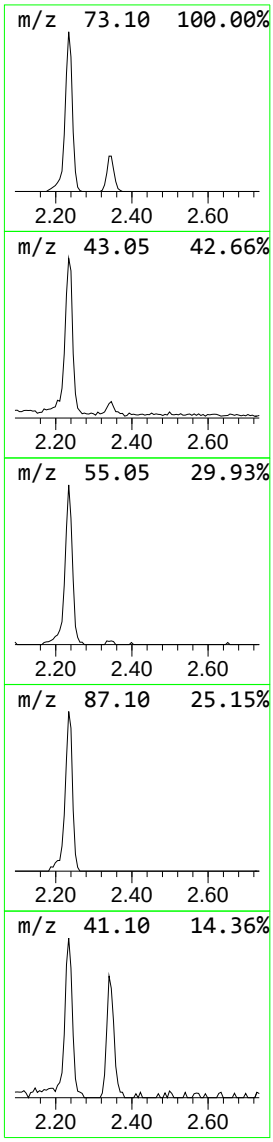
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	7.06 ng	164774	1,4-Dichlorobenzene-d4	6.887

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	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131126.D
Acq On : 10 Nov 2022 16:51
Operator : CG\JU
Sample : PB148948BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148948BL

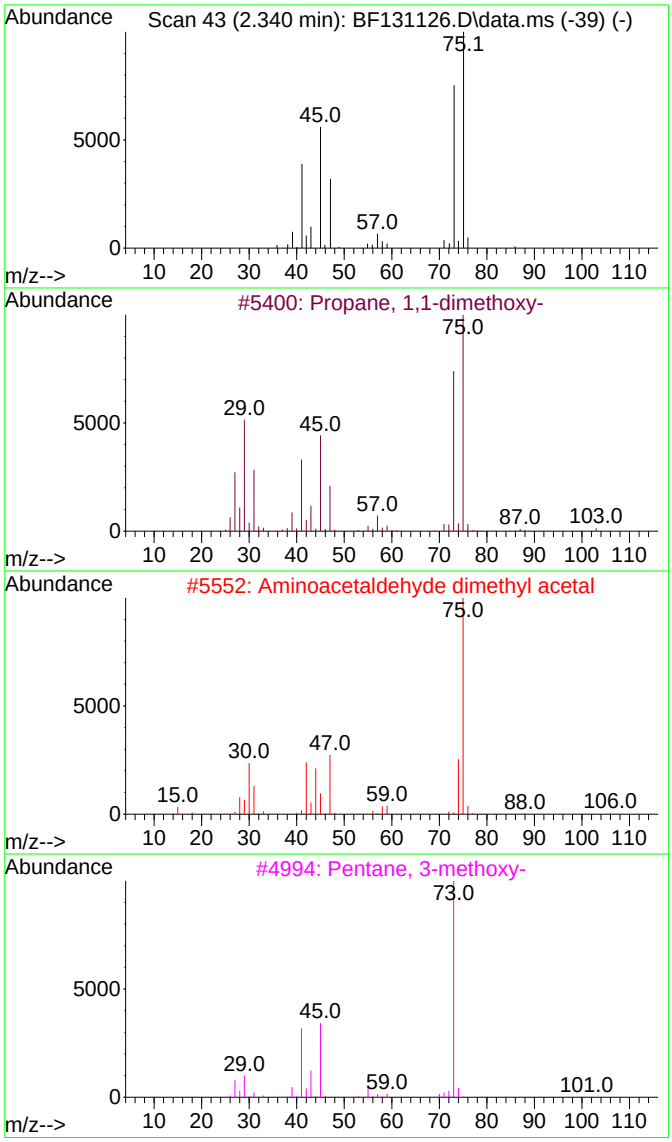
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

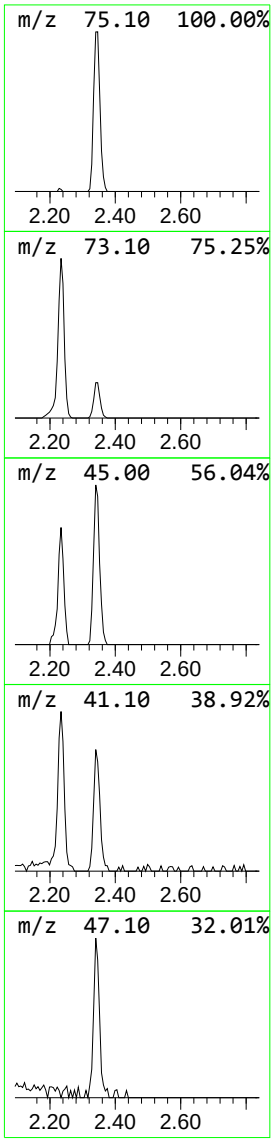
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.340	2.54 ng	59215	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	28
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16
4	2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	12
5	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131126.D
Acq On : 10 Nov 2022 16:51
Operator : CG\JU
Sample : PB148948BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148948BL

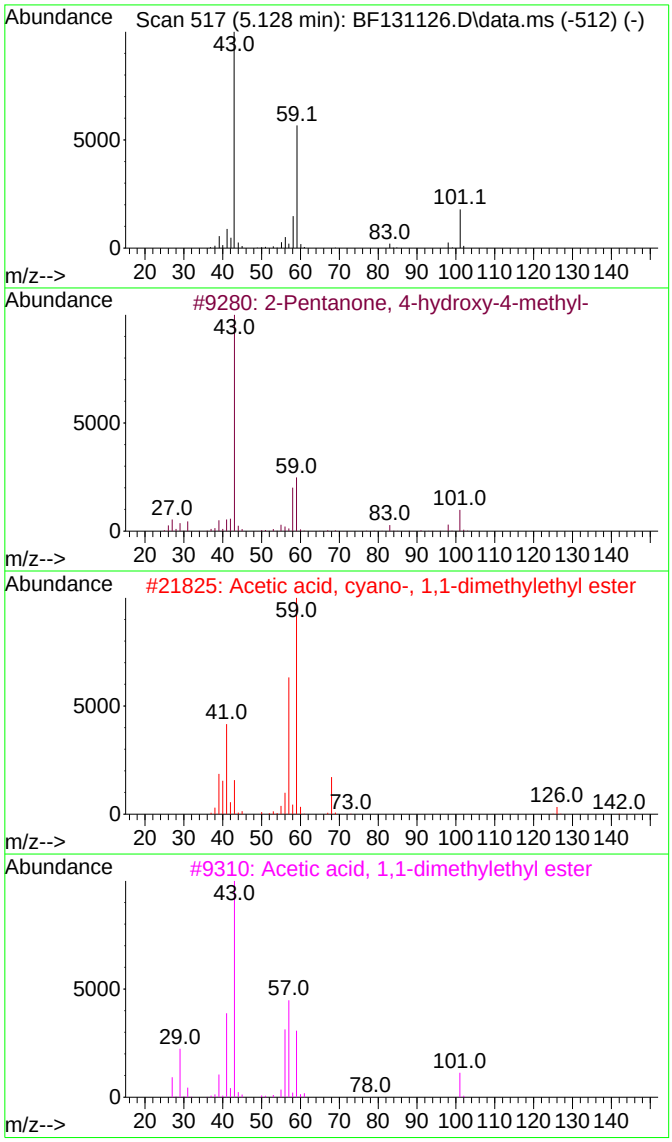
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

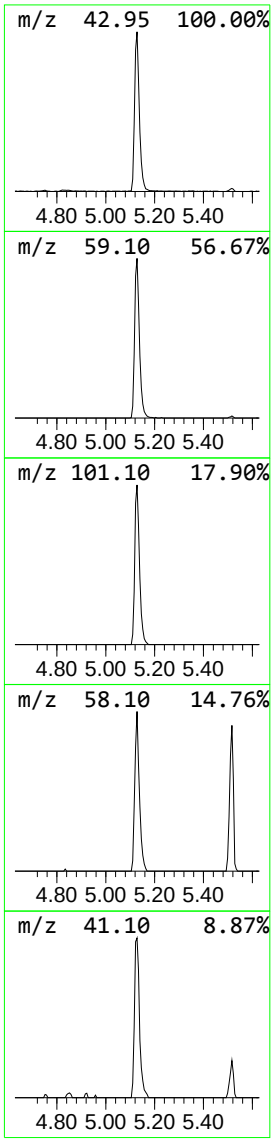
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.128	15.00 ng	349996	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131126.D
Acq On : 10 Nov 2022 16:51
Operator : CG\JU
Sample : PB148948BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148948BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

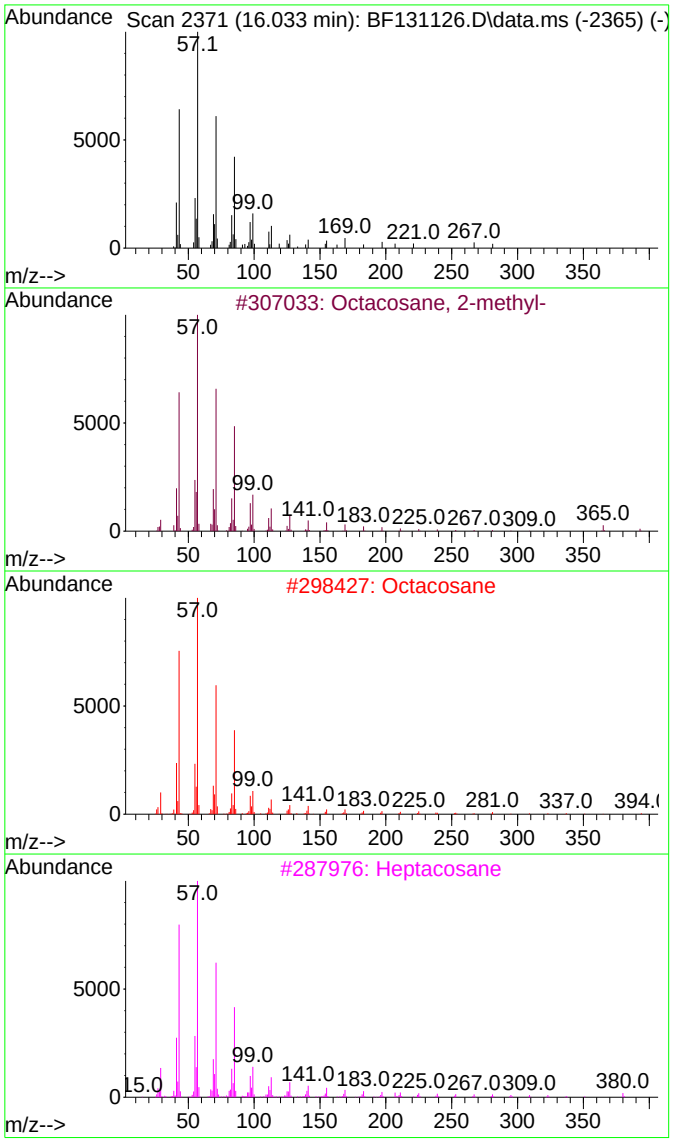
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

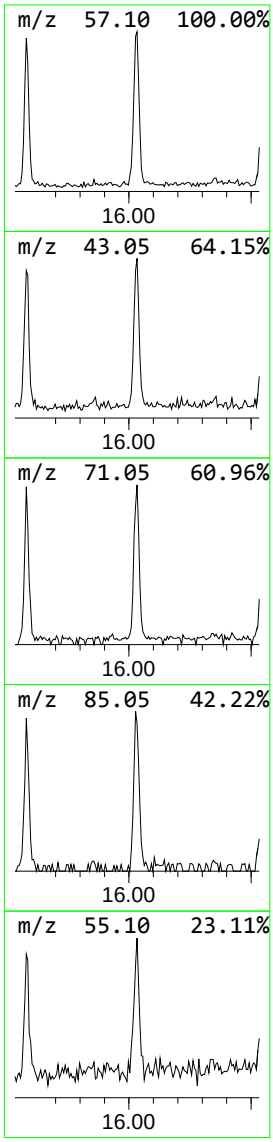
****

Peak Number 4 Octacosane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.033	2.82 ng	73512	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Hentriacontane	437	C31H64	000630-04-6	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131126.D
Acq On : 10 Nov 2022 16:51
Operator : CG\JU
Sample : PB148948BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148948BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

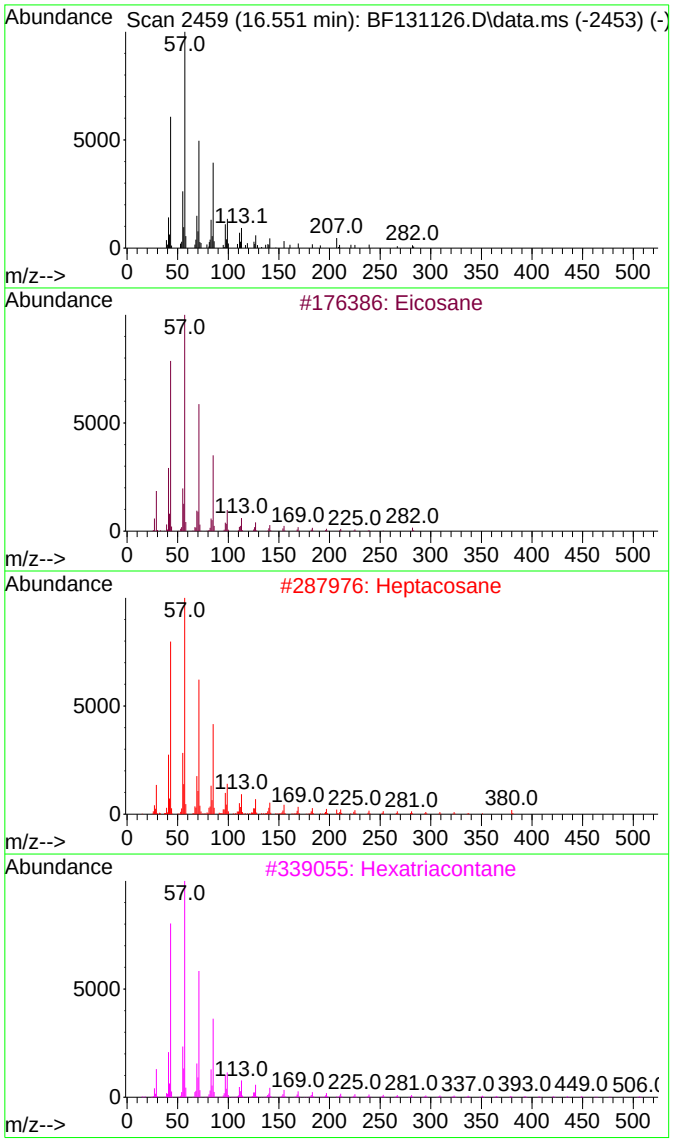
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

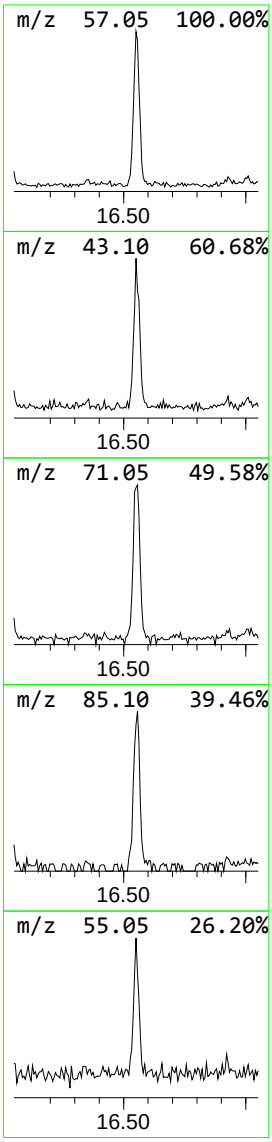
****

Peak Number 5 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.551	3.63 ng	94750	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	97
2	Heptacosane	380	C27H56	000593-49-7	90
3	Hexatriacontane	507	C36H74	000630-06-8	90
4	Octacosane	394	C28H58	000630-02-4	90
5	Heneicosane	296	C21H44	000629-94-7	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131126.D
Acq On : 10 Nov 2022 16:51
Operator : CG\JU
Sample : PB148948BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148948BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

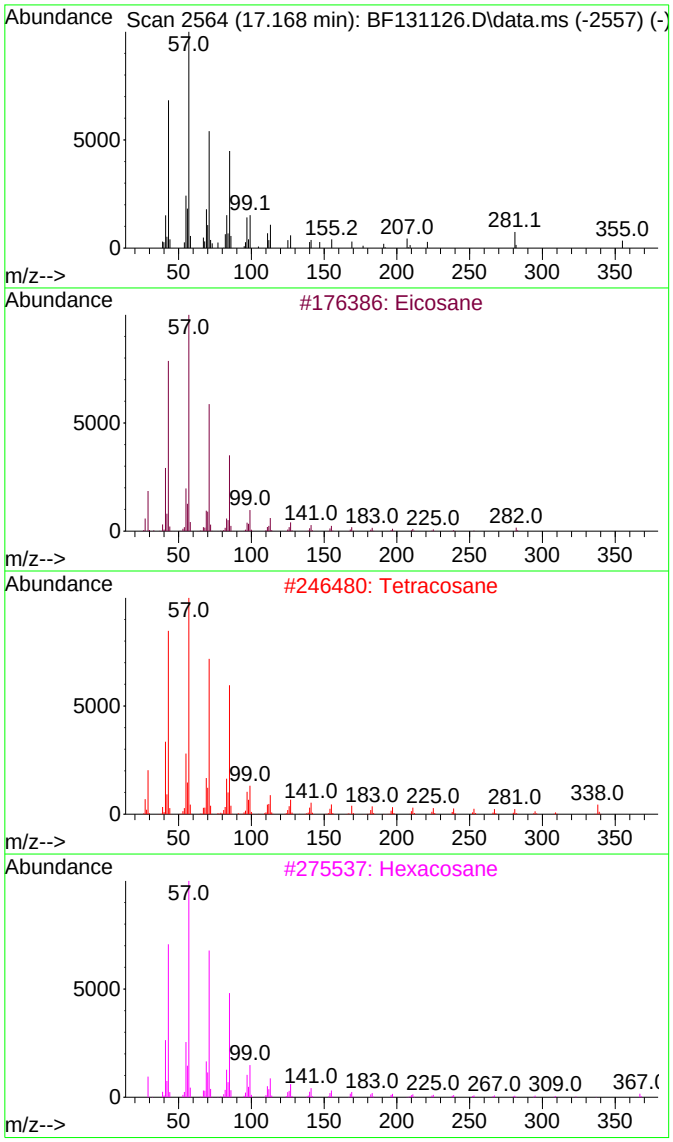
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

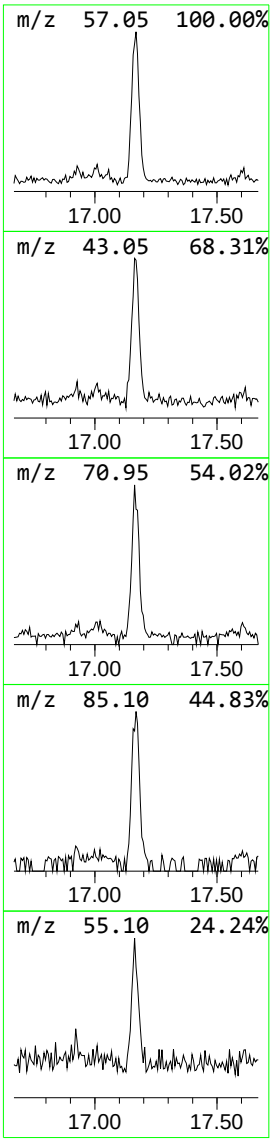
****

Peak Number 6 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.168	2.61 ng	68143	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	87
2	Tetracosane	338	C24H50	000646-31-1	86
3	Hexacosane	366	C26H54	000630-01-3	83
4	Tetratetracontane	619	C44H90	007098-22-8	83
5	Octacosane	394	C28H58	000630-02-4	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131126.D
Acq On : 10 Nov 2022 16:51
Operator : CG\JU
Sample : PB148948BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148948BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

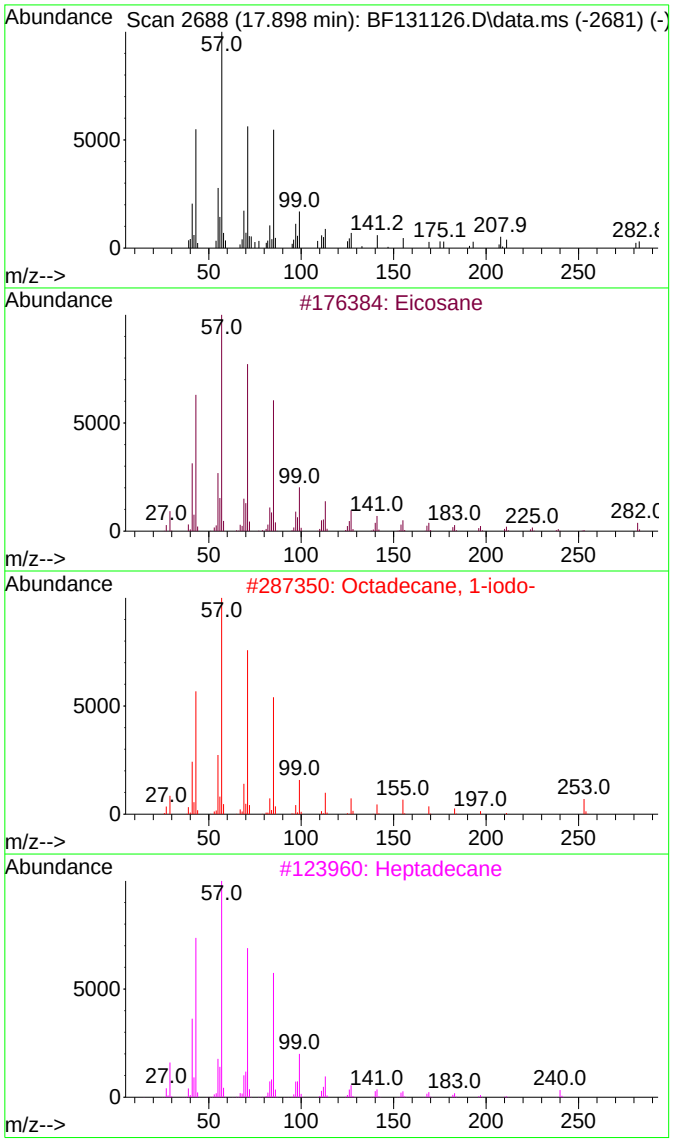
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

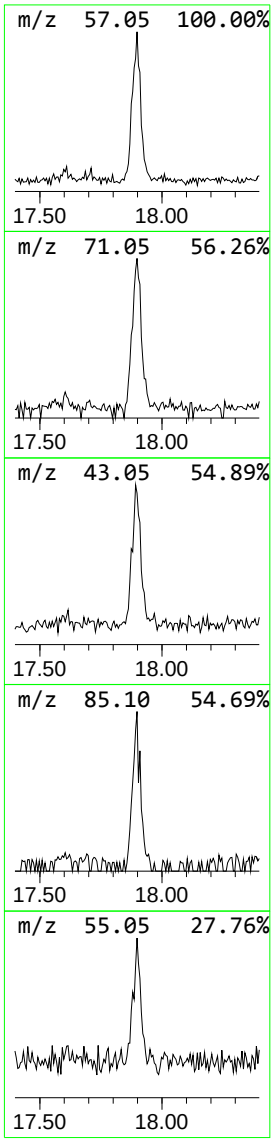
****

Peak Number 7 Octadecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.898	2.56 ng	66752	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	86
2	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
3	Heptadecane	240	C17H36	000629-78-7	80
4	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	80
5	Heneicosane, 5-methyl-	310	C22H46	025117-37-7	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131126.D
Acq On : 10 Nov 2022 16:51
Operator : CG\JU
Sample : PB148948BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148948BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

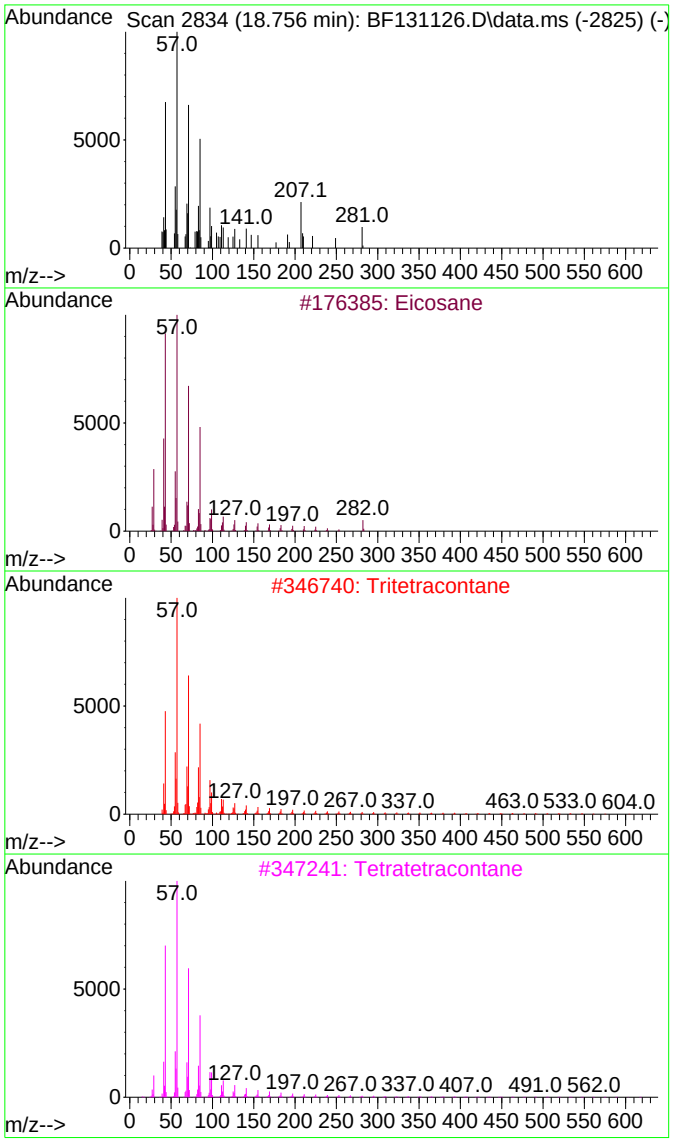
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

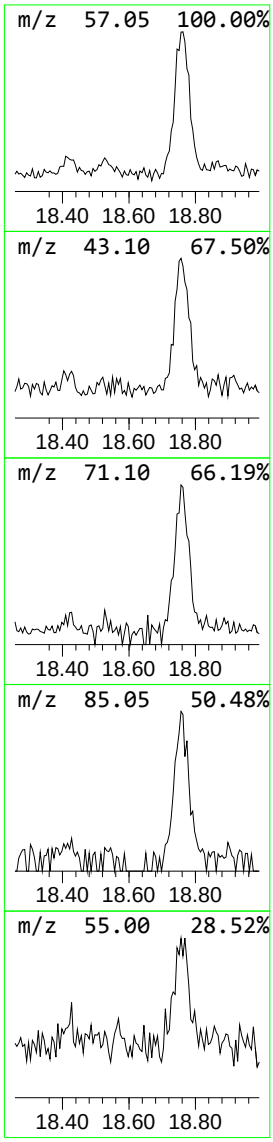
****

Peak Number 8 Tritetracontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.756	2.98 ng	77600	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	83
2	Tritetracontane	605	C43H88	007098-21-7	64
3	Tetratetracontane	619	C44H90	007098-22-8	64
4	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	64
5	Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111022\
Data File : BF131126.D
Acq On : 10 Nov 2022 16:51
Operator : CG\JU
Sample : PB148948BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB148948BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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...	2.234	7.1	ng	164774	1	6.887	466803	20.0
Propane, 1,1-di...	2.340	2.5	ng	59215	1	6.887	466803	20.0
2-Pentanone, 4-...	5.128	15.0	ng	349996	1	6.887	466803	20.0
Octacosane, 2-m...	16.033	2.8	ng	73512	6	15.574	521608	20.0
Eicosane	16.551	3.6	ng	94750	6	15.574	521608	20.0
Tetracosane	17.168	2.6	ng	68143	6	15.574	521608	20.0
Octadecane, 1-i...	17.898	2.6	ng	66752	6	15.574	521608	20.0
Tritetracontane	18.756	3.0	ng	77600	6	15.574	521608	20.0