LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010523\
Data File : BF131923.D
Acq On : 05 Jan 2023 19:32
Operator : CG\JU
Sample : 01029-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-204

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-BF122422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131923.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	11	rVB	35524	41731	1.98%	0.283%
2	4.999	490	495	509	rVB	529689	677828	32.20%	4.595%
3	5.410	561	565	569	rBV	1724302	1597779	75.90%	10.832%
4	6.434	735	739	742	rBV	1582998	1662264	78.96%	11.269%
5	6.798	798	801	805	rBV	509593	413184	19.63%	2.801%
6	7.369	893	898	901	rBV	1082832	1087387	51.65%	7.372%
7	8.092	1016	1021	1024	rBV	597111	528591	25.11%	3.583%
8	9.175	1199	1205	1208	rBV	2373059	2052145	97.48%	13.912%
9	9.851	1316	1320	1324	rBV	777466	631299	29.99%	4.280%
10	9.986	1340	1343	1353	rBV	97862	86374	4.10%	0.586%
11	10.575	1439	1443	1446	rVB	615770	498564	23.68%	3.380%
12	10.645	1451	1455	1459	rBV	1490137	1412481	67.09%	9.575%
13	11.345	1570	1574	1577	rBV	862456	683347	32.46%	4.633%
14	11.880	1661	1665	1668	rBV	83120	81047	3.85%	0.549%
15	12.127	1703	1707	1713	rVB	53901	45828	2.18%	0.311%
16	12.945	1841	1846	1849	rBV	2391018	2105225	100.00%	14.272%
17	13.422	1922	1927	1931	rBV	72128	63546	3.02%	0.431%
18	13.839	1995	1998	2014	rBV	153930	237038	11.26%	1.607%
19	13.998	2022	2025	2029	rVB	461110	407795	19.37%	2.765%
20	14.492	2106	2109	2117	rVB5	12210	24693	1.17%	0.167%
21	14.851	2166	2170	2173	rBV	24262	24082	1.14%	0.163%
22	15.474	2271	2276	2283	rBV	282675	350272	16.64%	2.375%
23	16.004	2359	2366	2370	rBV10	16232	38567	1.83%	0.261%

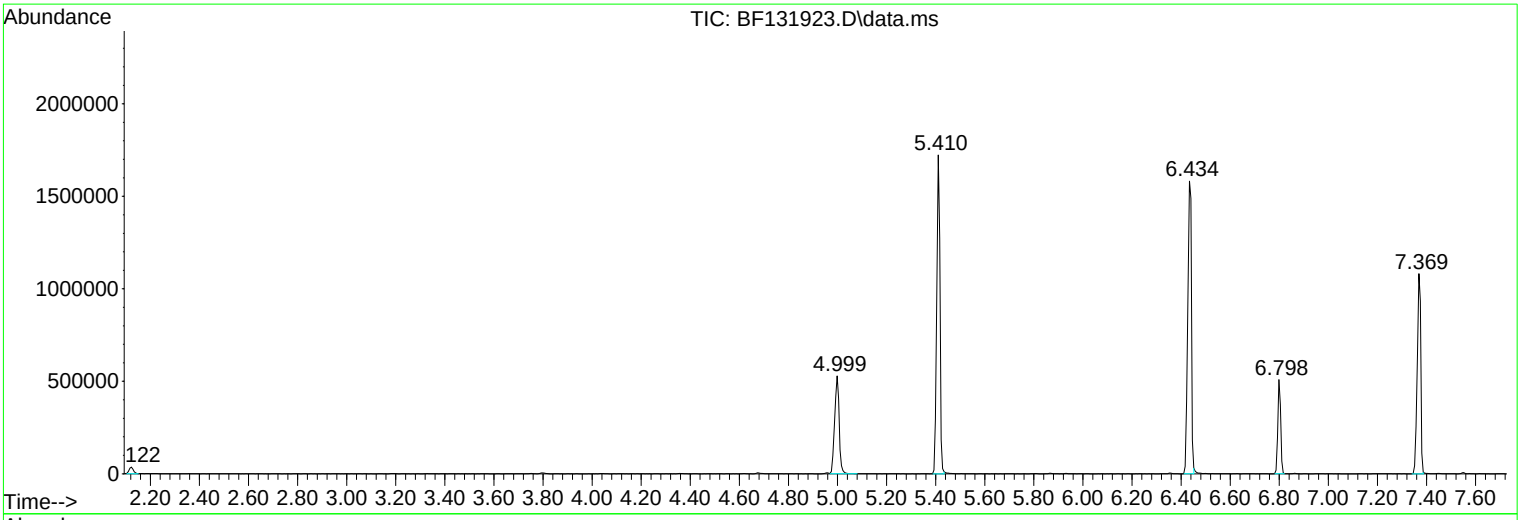
Sum of corrected areas: 14751067

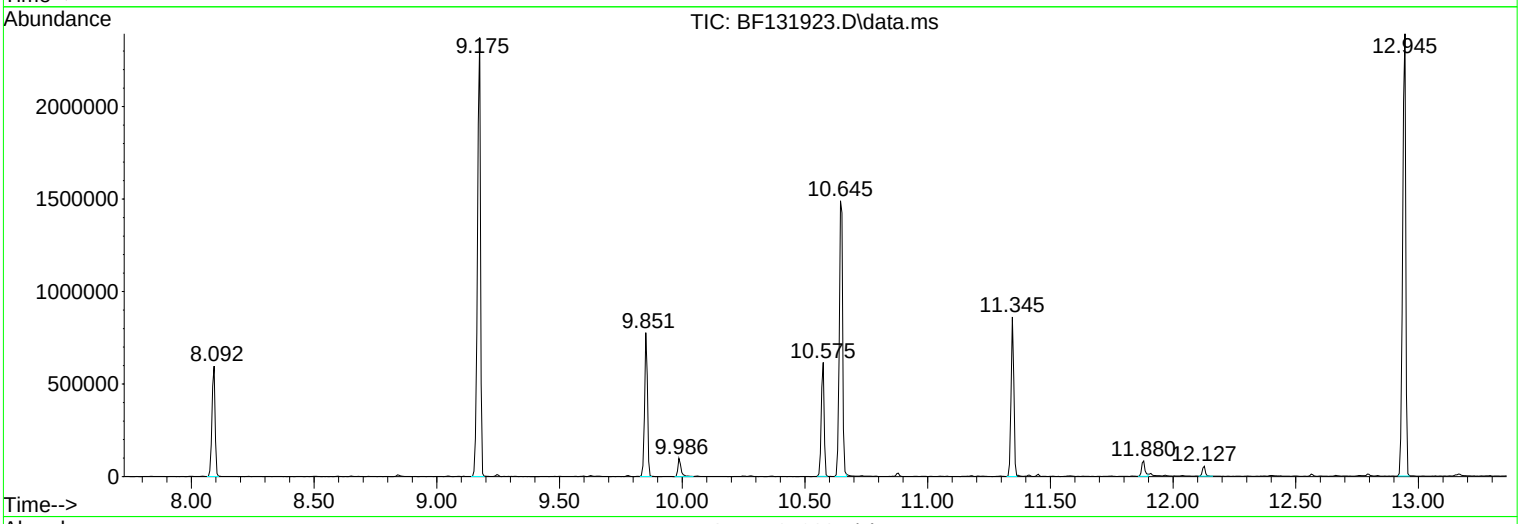
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010523\
Data File : BF131923.D
Acq On : 05 Jan 2023 19:32
Operator : CG\JU
Sample : 01029-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

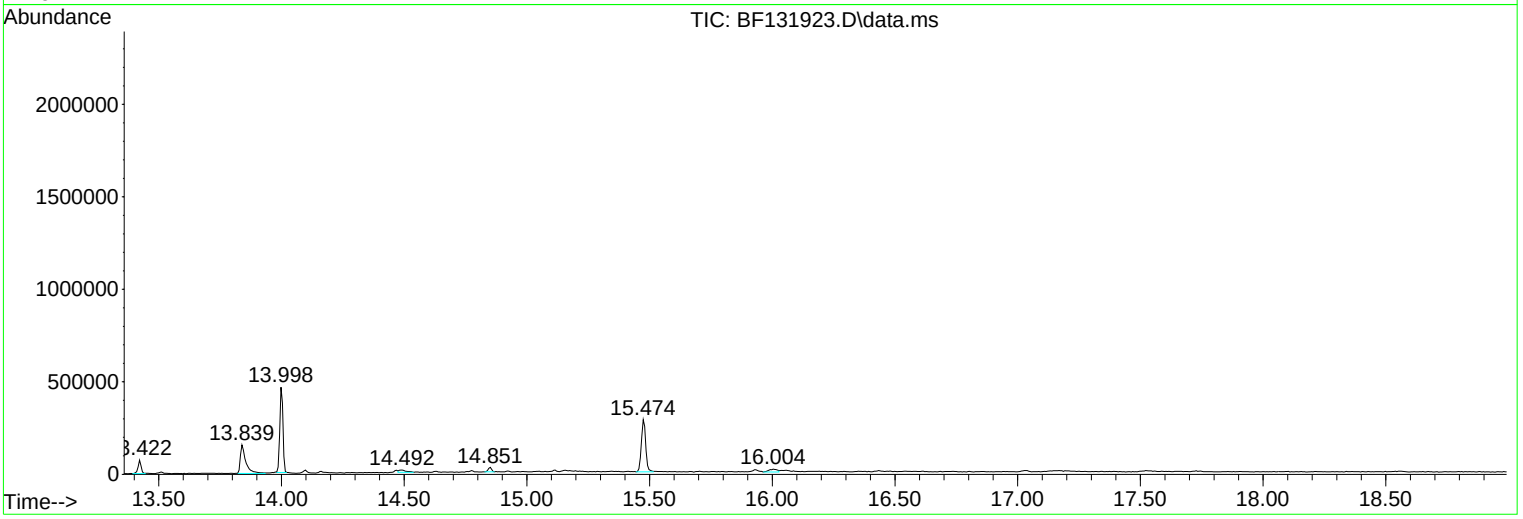
Instrument :
BNA_F
ClientSampleId :
TP-204

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.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 : BF131923.D
Acq On : 05 Jan 2023 19:32
Operator : CG\JU
Sample : 01029-04
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

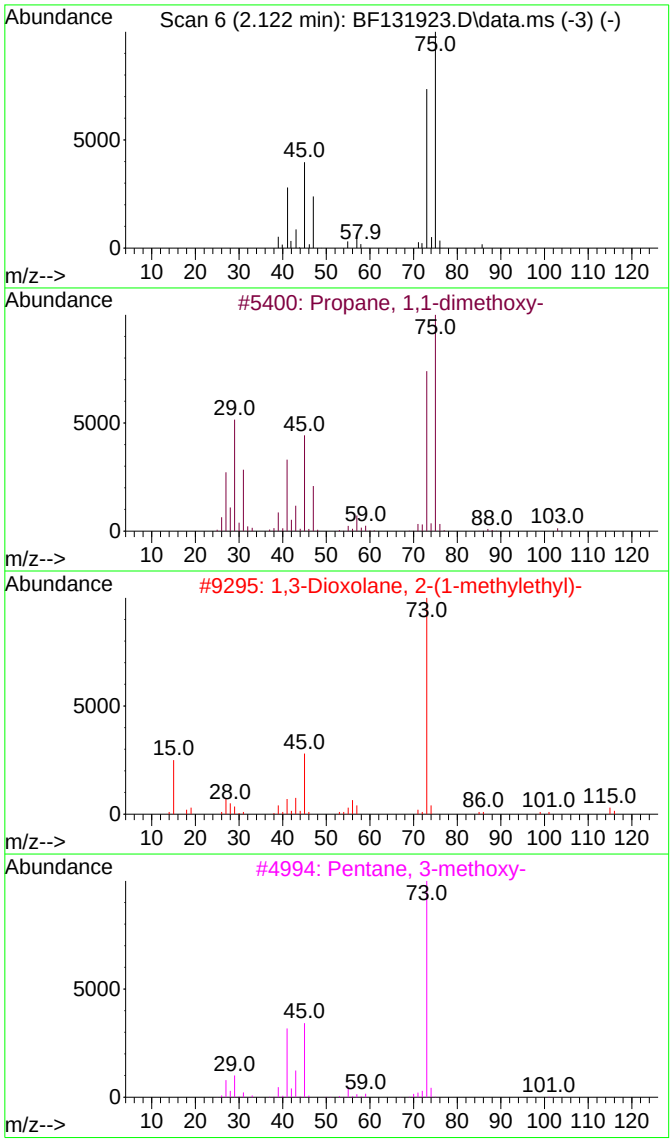
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

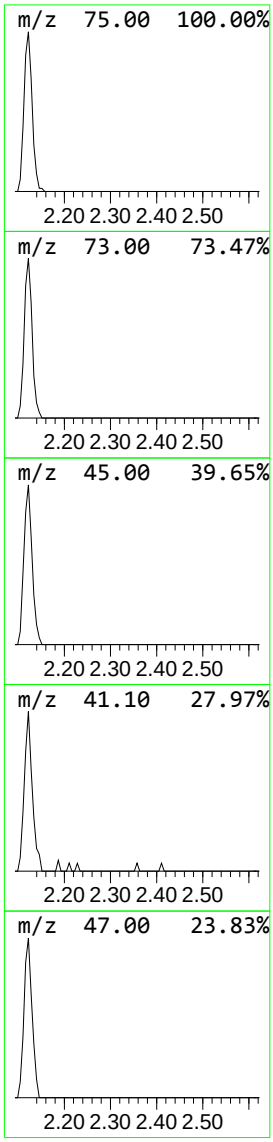
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	2.02 ng	41731	1,4-Dichlorobenzene-d4	6.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	27
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
4	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9





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Data File : BF131923.D
Acq On : 05 Jan 2023 19:32
Operator : CG\JU
Sample : 01029-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-204

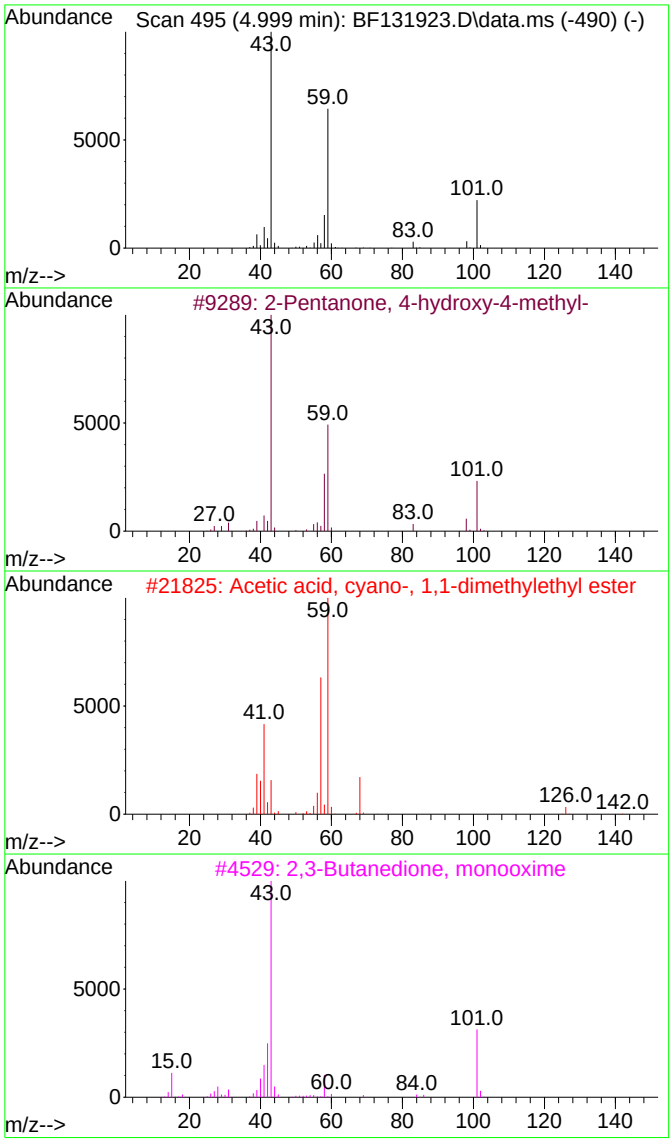
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

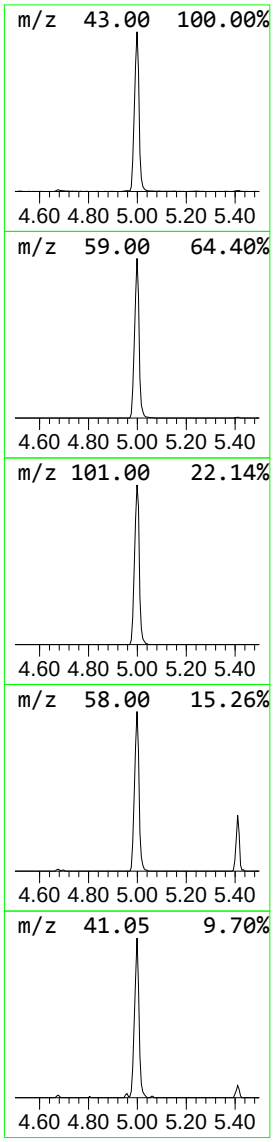
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.999	32.81 ng	677828	1,4-Dichlorobenzene-d4	6.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF131923.D
Acq On : 05 Jan 2023 19:32
Operator : CG\JU
Sample : 01029-04
Misc :
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Instrument :
BNA_F
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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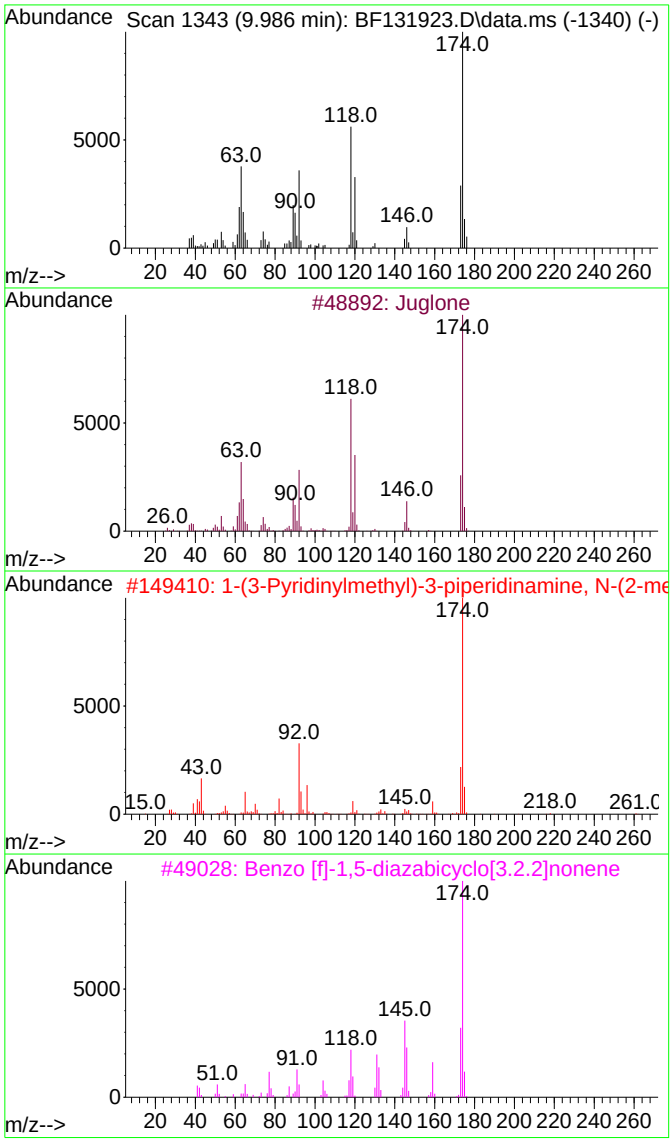
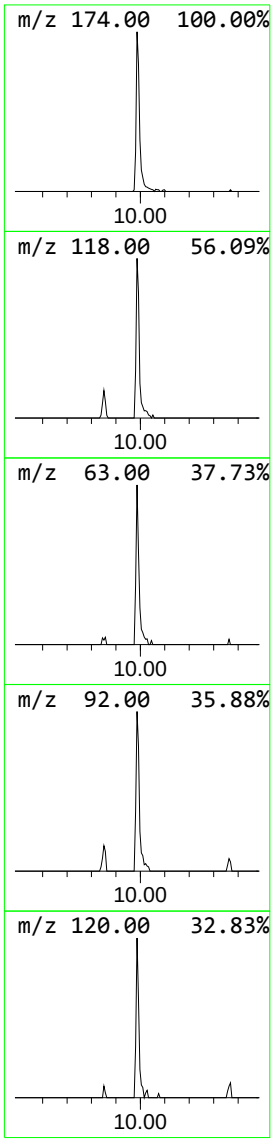
****

Peak Number 3 Juglone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.986	2.74 ng	86374	Acenaphthene-d10	9.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Juglone	174	C10H6O3	000481-39-0	94
2	1-(3-Pyridinylmethyl)-3-piperidi...	261	C15H23N3O	1000469-14-1	38
3	Benzo [f]-1,5-diazabicyclo[3.2.2...	174	C11H14N2	007092-76-4	35
4	Benzene, 2,4-diisocyanato-1-methyl-	174	C9H6N2O2	000584-84-9	35
5	6-Methylquinazolin-4(3H)-one, Me...	174	C10H10N2O	1010504-83-5	32





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Data File : BF131923.D
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Operator : CG\JU
Sample : 01029-04
Misc :
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Instrument :
BNA_F
ClientSampleId :
TP-204

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

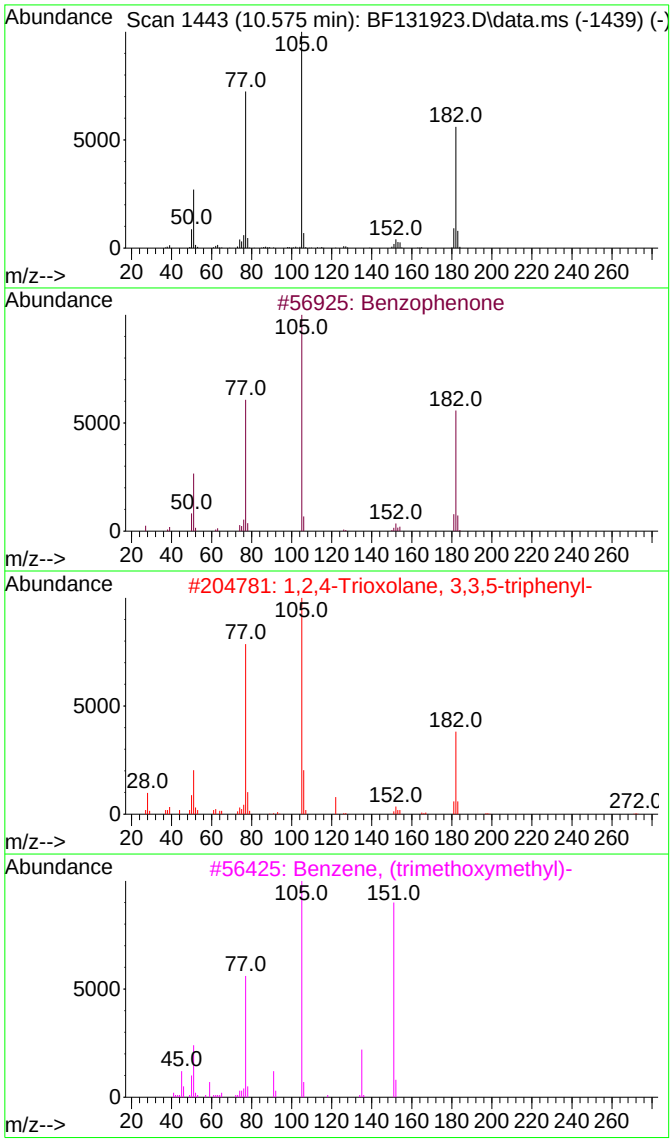
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

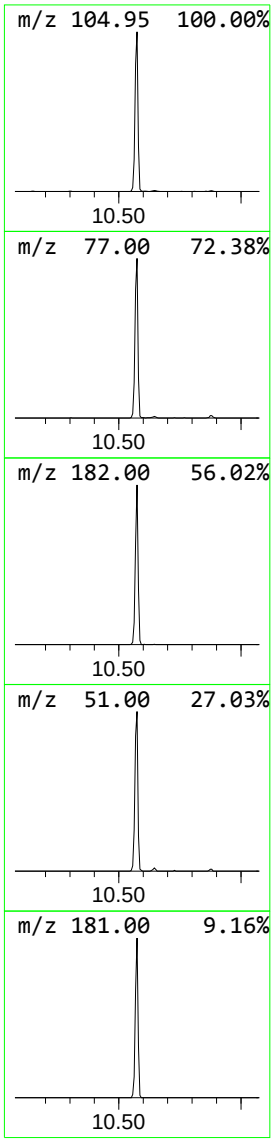
****

Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.575	15.79 ng	498564	Acenaphthene-d10	9.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	64
3	Benzene, (trimethoxymethyl)-	182	C10H14O3	000707-07-3	47
4	2-Chloro-1-phenyl-1-propanone	168	C9H9ClO	006084-17-9	47
5	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47





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Operator : CG\JU
Sample : 01029-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-204

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

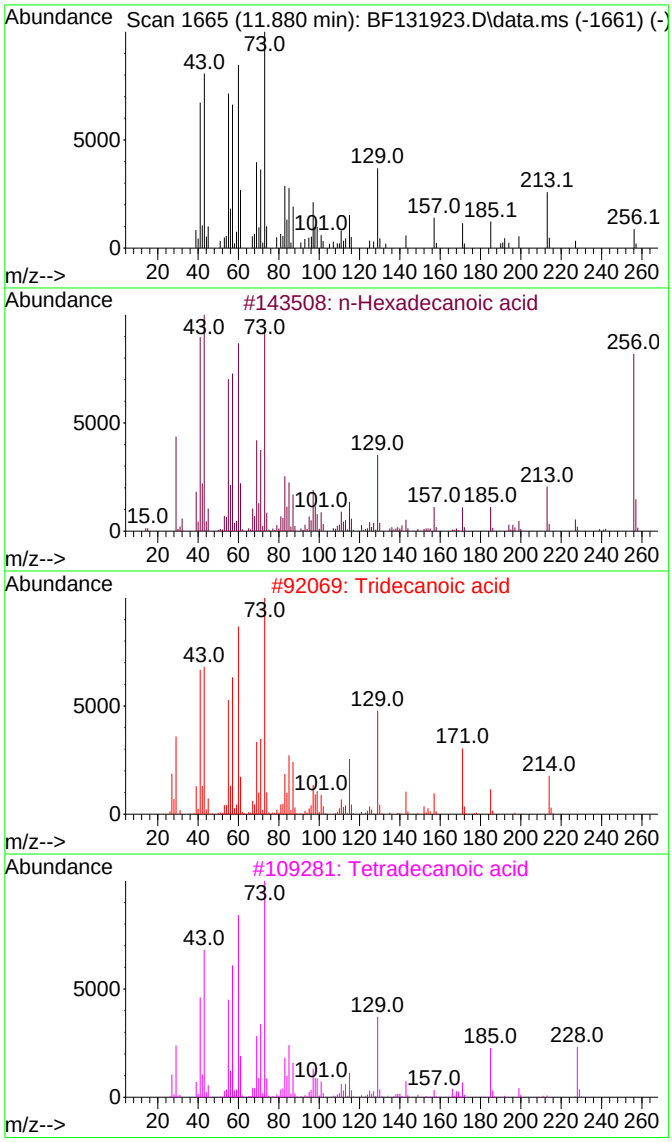
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

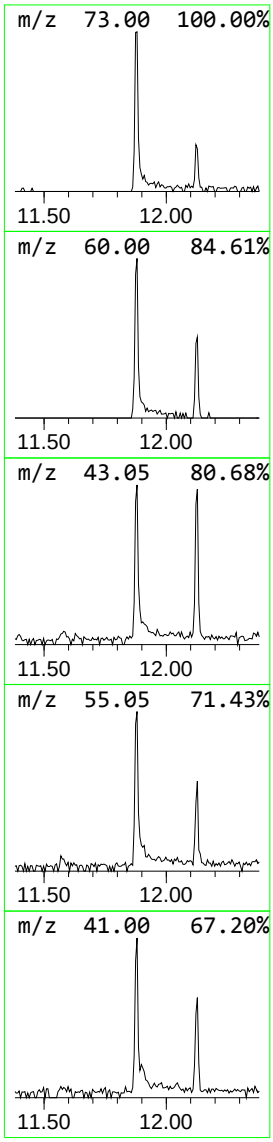
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	2.37 ng	81047	Phenanthrene-d10	11.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Dodecanoic acid	200	C12H24O2	000143-07-7	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





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Data File : BF131923.D
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Operator : CG\JU
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BNA_F
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TP-204

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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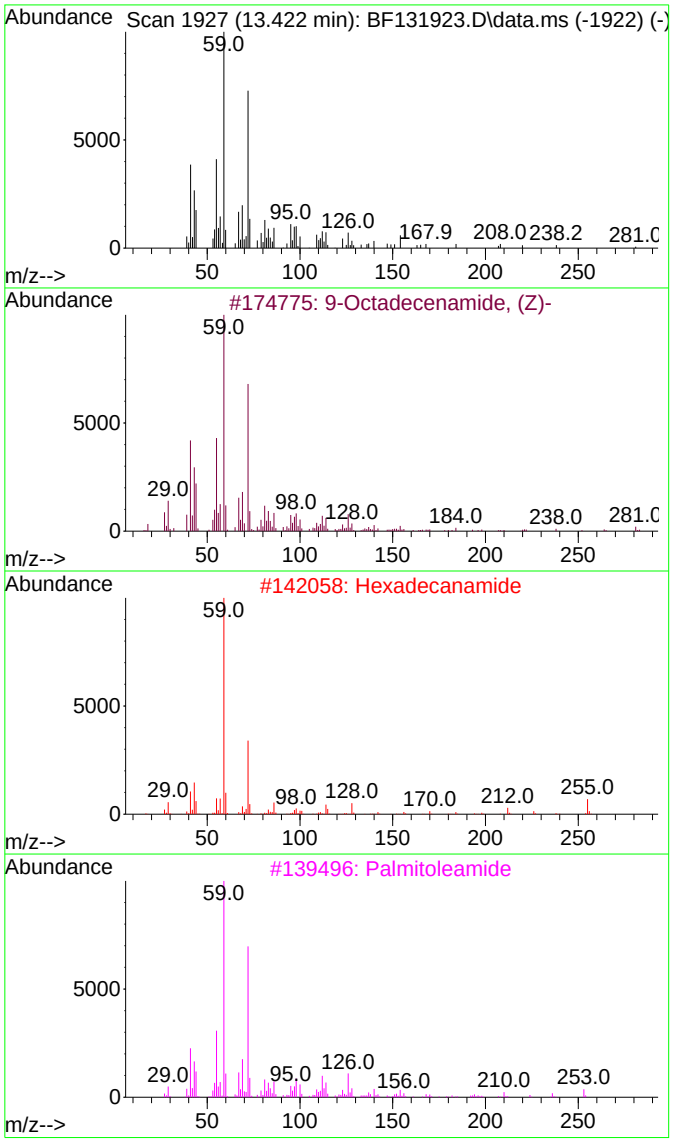
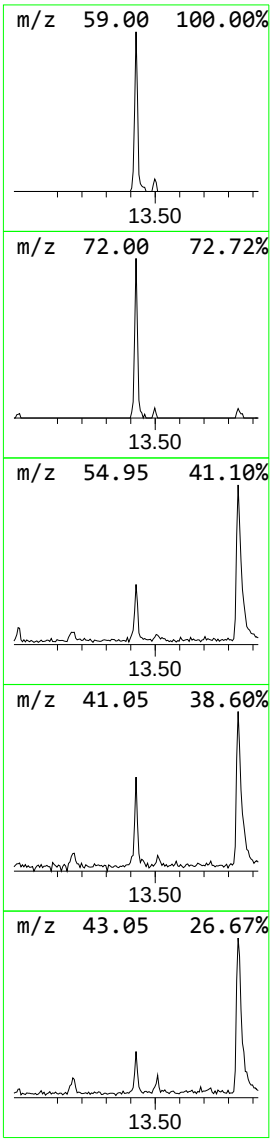
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.422	3.12 ng	63546	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Hexadecanamide	255	C16H33NO	000629-54-9	64
3	Palmitoleamide	253	C16H31NO	106010-22-4	59
4	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	53
5	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010523\
Data File : BF131923.D
Acq On : 05 Jan 2023 19:32
Operator : CG\JU
Sample : 01029-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-204

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

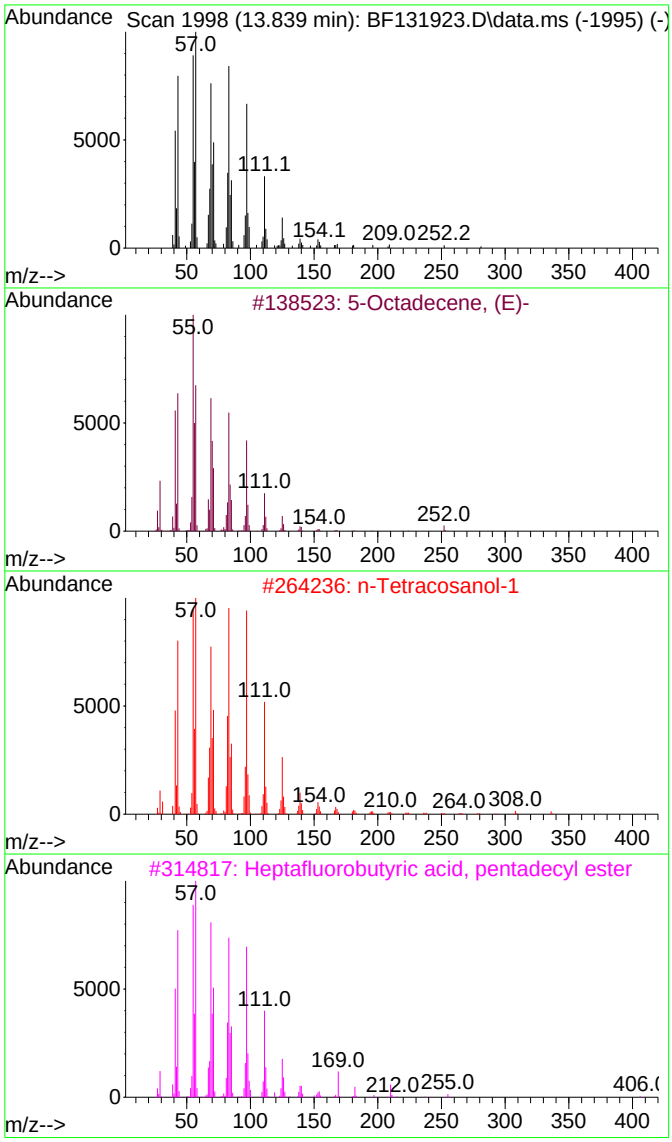
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

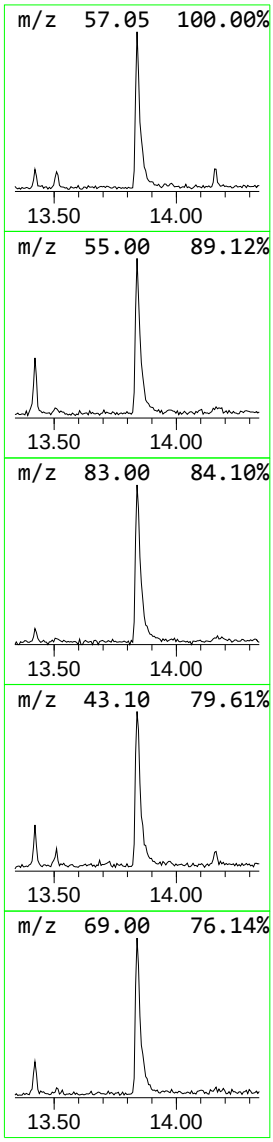
****

Peak Number 7 5-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	11.63 ng	237038	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	1-Nonadecene	266	C19H38	018435-45-5	91





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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
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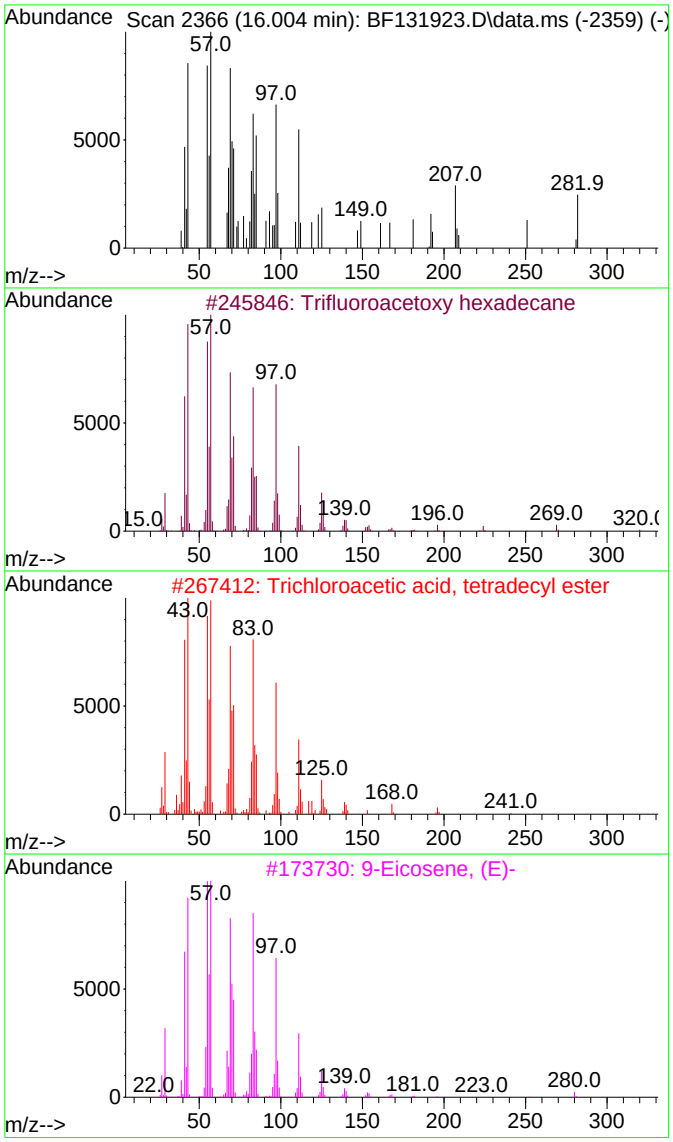
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

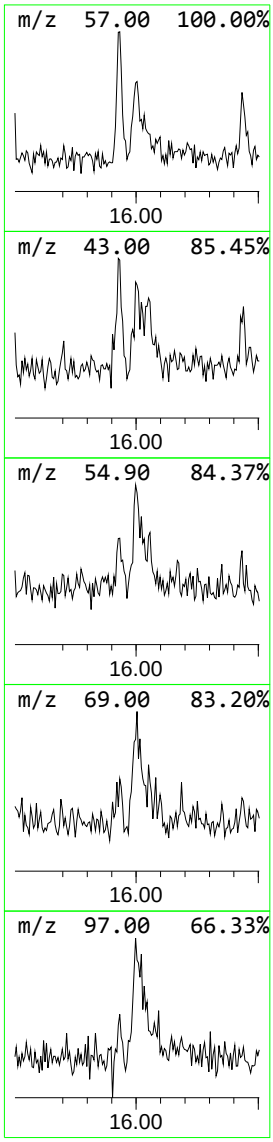
****

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.004	2.20 ng	38567	Perylene-d12	15.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	58
2	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	55
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	55
4	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	55
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	53





Tentatively Identified Compound (LSC) summary

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Data File : BF131923.D
Acq On : 05 Jan 2023 19:32
Operator : CG\JU
Sample : 01029-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-204

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.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
Propane, 1,1-di...	2.122	2.0	ng	41731	1	6.798	413184	20.0
2-Pentanone, 4-...	4.999	32.8	ng	677828	1	6.798	413184	20.0
Juglone	9.986	2.7	ng	86374	3	9.851	631299	20.0
Benzophenone	10.575	15.8	ng	498564	3	9.851	631299	20.0
n-Hexadecanoic ...	11.880	2.4	ng	81047	4	11.345	683347	20.0
9-Octadecenamid...	13.422	3.1	ng	63546	5	13.998	407795	20.0
5-Octadecene, (E)-	13.839	11.6	ng	237038	5	13.998	407795	20.0
Trifluoroacetox...	16.004	2.2	ng	38567	6	15.474	350272	20.0