LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122022\
Data File : BF131727.D
Acq On : 20 Dec 2022 22:45
Operator : CG\JU
Sample : N6071-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FVSUB-TP8-COMP-08

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-BF122022.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131727.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	3	14	24	rVB	259053	392337	9.25%	1.491%
2	5.093	506	511	526	rVB	368324	577218	13.62%	2.194%
3	5.493	573	579	582	rBV	3279647	3588619	84.65%	13.639%
4	6.504	744	751	753	rBV	2998177	3709352	87.50%	14.098%
5	6.863	808	812	815	rBV	611525	477233	11.26%	1.814%
6	7.440	903	910	912	rBV	1965607	2394052	56.47%	9.099%
7	8.151	1026	1031	1035	rBV	669232	615155	14.51%	2.338%
8	9.239	1209	1216	1219	rBV	4327521	4239349	100.00%	16.112%
9	9.916	1326	1331	1334	rBV	911330	738808	17.43%	2.808%
10	10.633	1446	1453	1457	rBV	308727	250607	5.91%	0.952%
11	10.710	1460	1466	1469	rBV	2816755	2749323	64.85%	10.449%
12	11.410	1581	1585	1588	rBV	904139	793570	18.72%	3.016%
13	11.933	1671	1674	1677	rBV2	71353	60438	1.43%	0.230%
14	13.004	1851	1856	1859	rBV	4056920	4215585	99.44%	16.022%
15	13.427	1925	1928	1932	rBV	311208	294462	6.95%	1.119%
16	13.474	1932	1936	1943	rVB2	58119	77049	1.82%	0.293%
17	13.898	2004	2008	2020	rBV	111426	198400	4.68%	0.754%
18	14.057	2031	2035	2038	rBV	523655	453089	10.69%	1.722%
19	14.821	2159	2165	2171	rBV2	46219	62507	1.47%	0.238%
20	15.551	2284	2289	2298	rBV2	330598	424010	10.00%	1.612%

Sum of corrected areas: 26311163

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122022\
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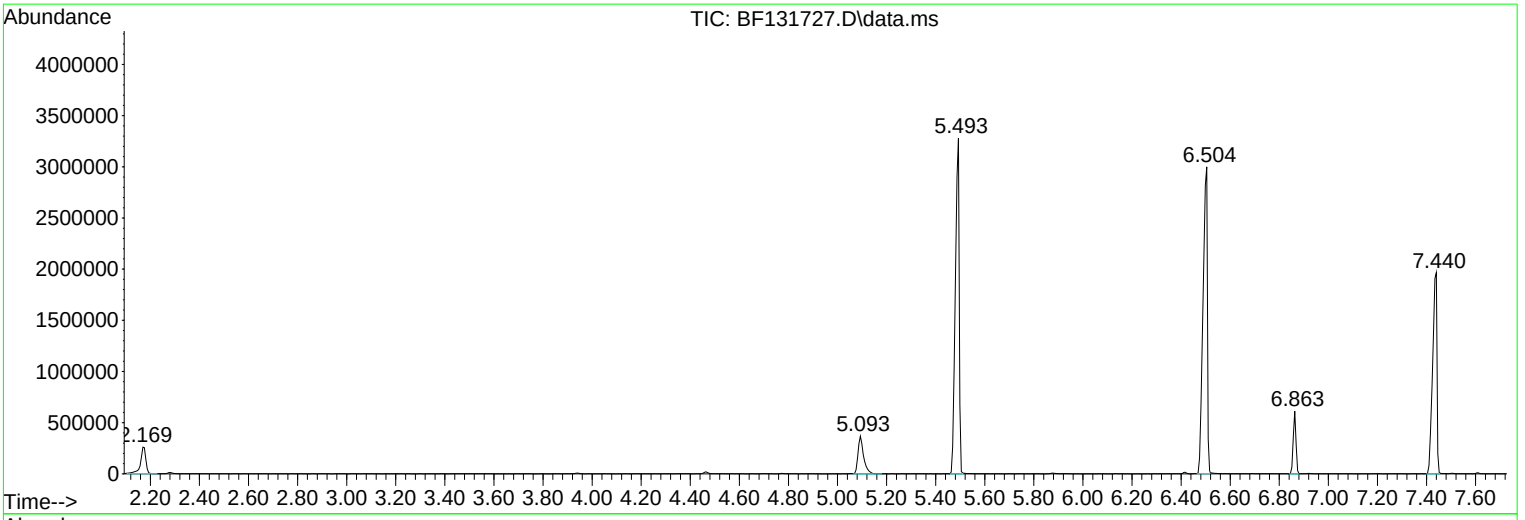
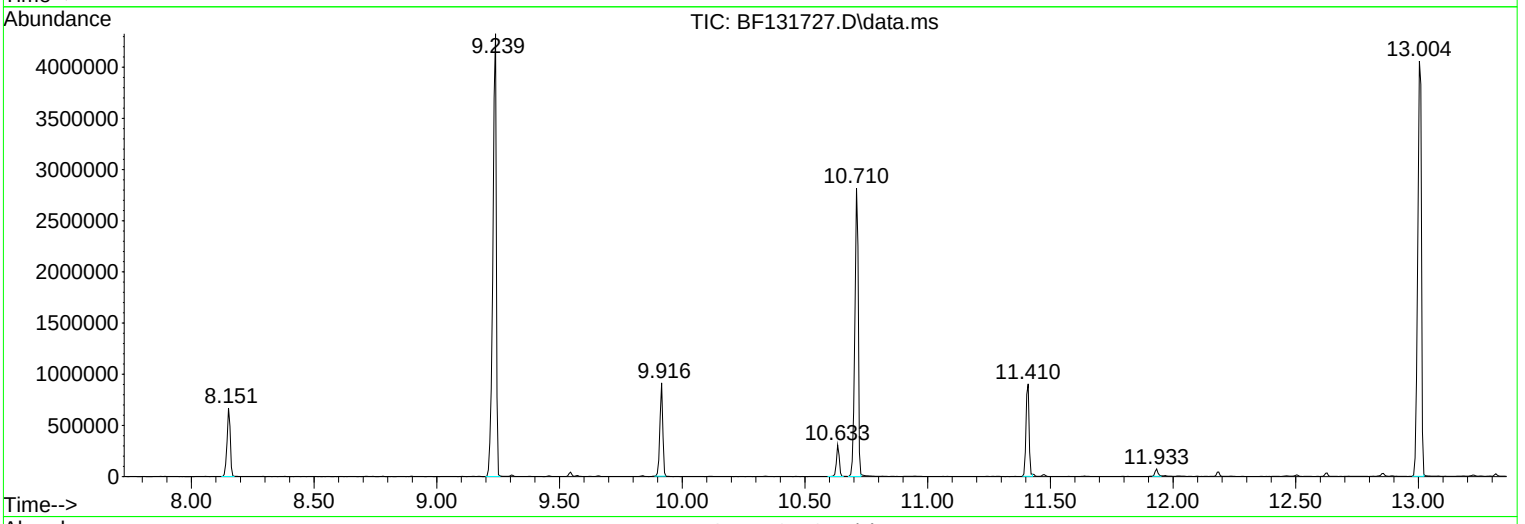
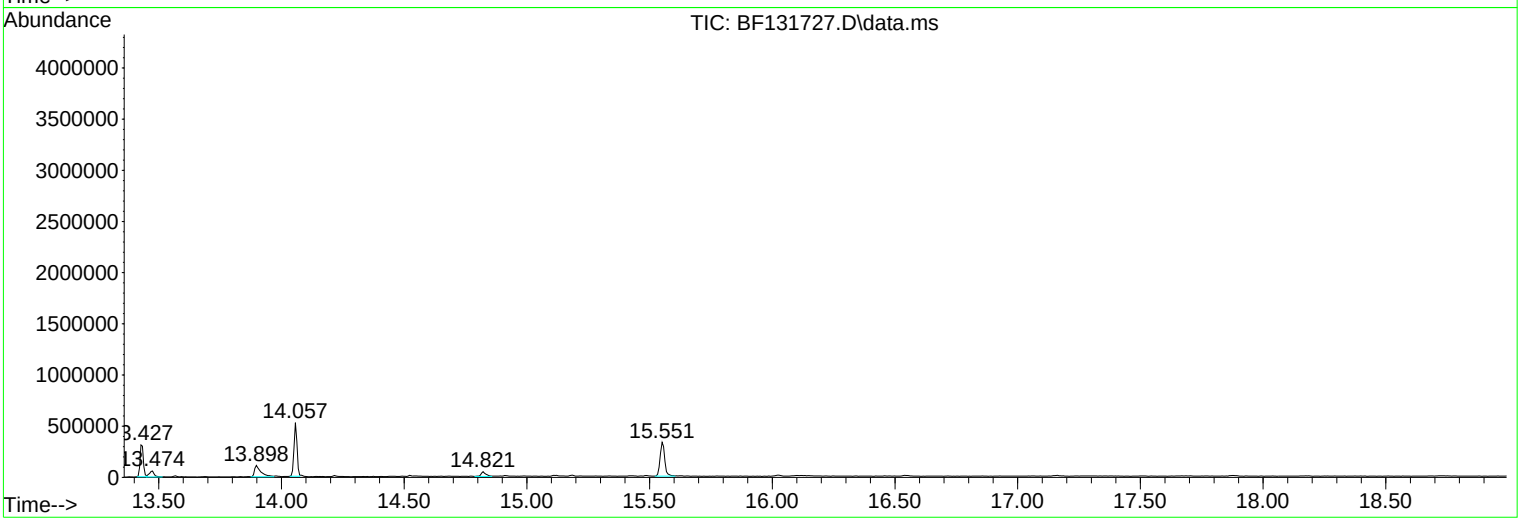
BNA_F
ClientSampleId :
FVSUB-TP8-COMP-08

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.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 : BF131727.D
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Operator : CG\JU
Sample : N6071-11
Misc :
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Instrument :
BNA_F
ClientSampleId :
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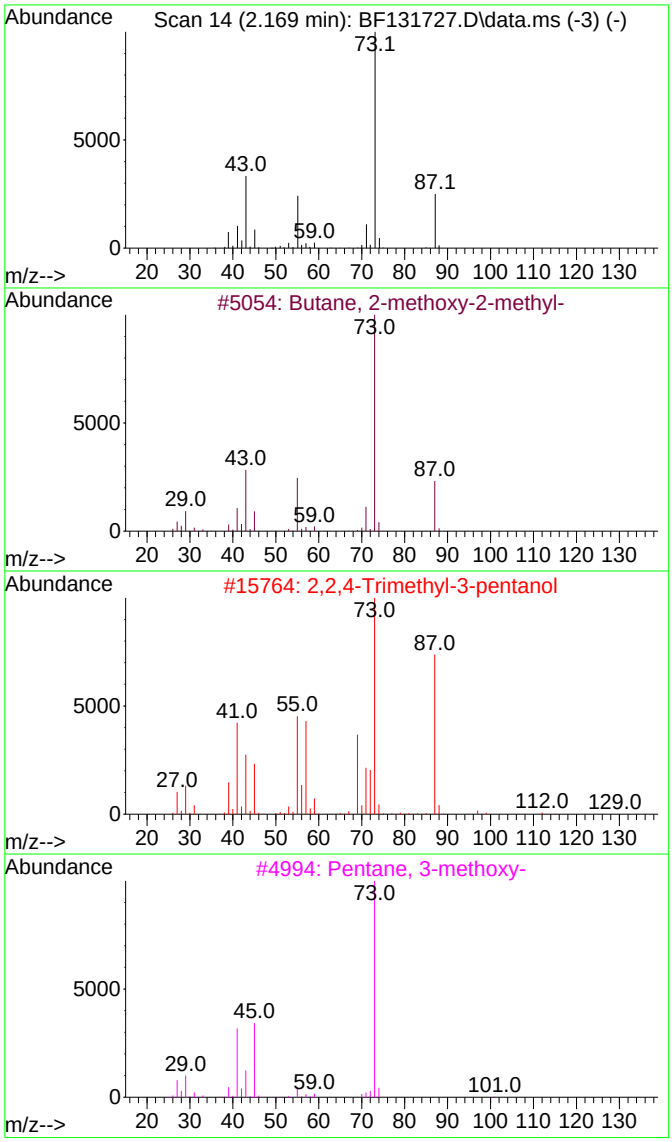
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

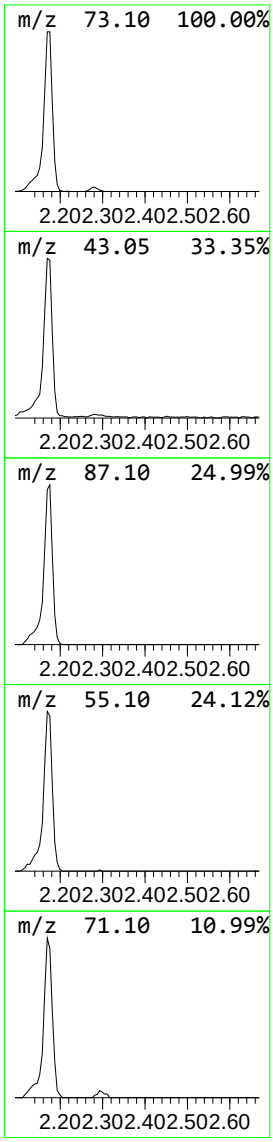
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	16.44 ng	392337	1,4-Dichlorobenzene-d4	6.863

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	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Data File : BF131727.D
Acq On : 20 Dec 2022 22:45
Operator : CG\JU
Sample : N6071-11
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Instrument :
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ClientSampleId :
FVSUB-TP8-COMP-08

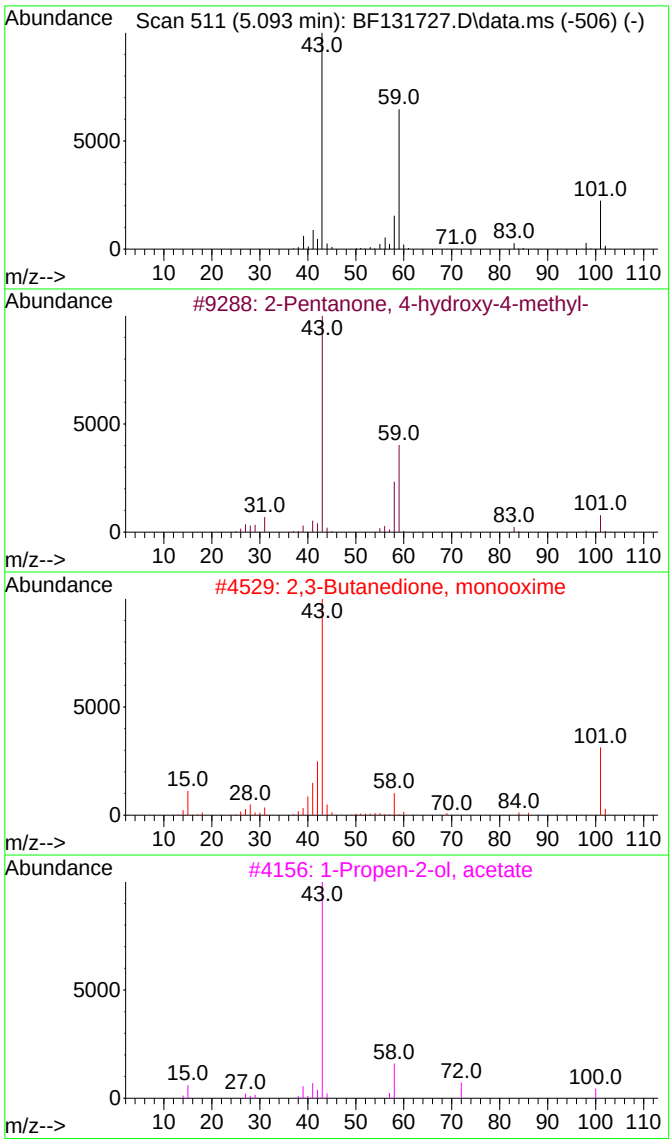
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

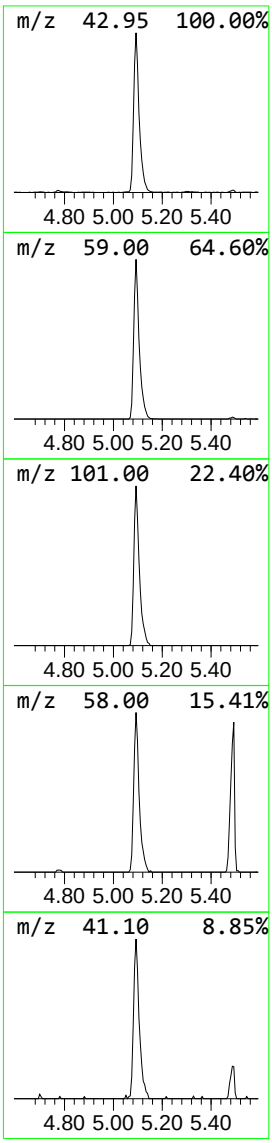
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	24.19 ng	577218	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Guanidine	59	CH5N3	000113-00-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122022\
Data File : BF131727.D
Acq On : 20 Dec 2022 22:45
Operator : CG\JU
Sample : N6071-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FVSUB-TP8-COMP-08

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

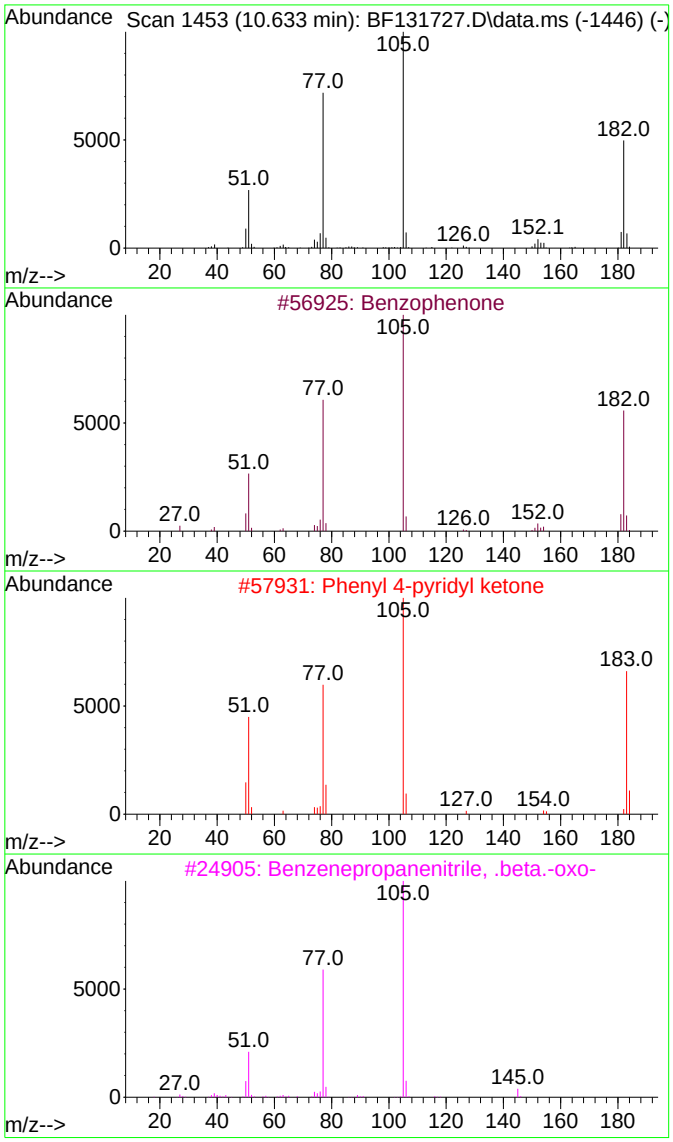
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

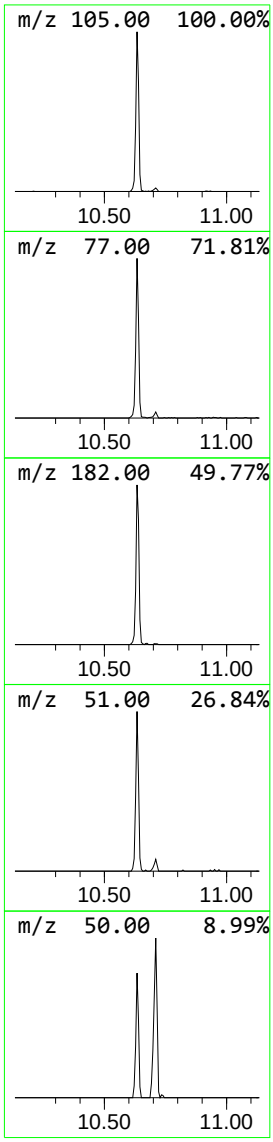
****

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.634	6.78 ng	250607	Acenaphthene-d10	9.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
3	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
4	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
5	2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47





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Acq On : 20 Dec 2022 22:45
Operator : CG\JU
Sample : N6071-11
Misc :
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Instrument :
BNA_F
ClientSampleId :
FVSUB-TP8-COMP-08

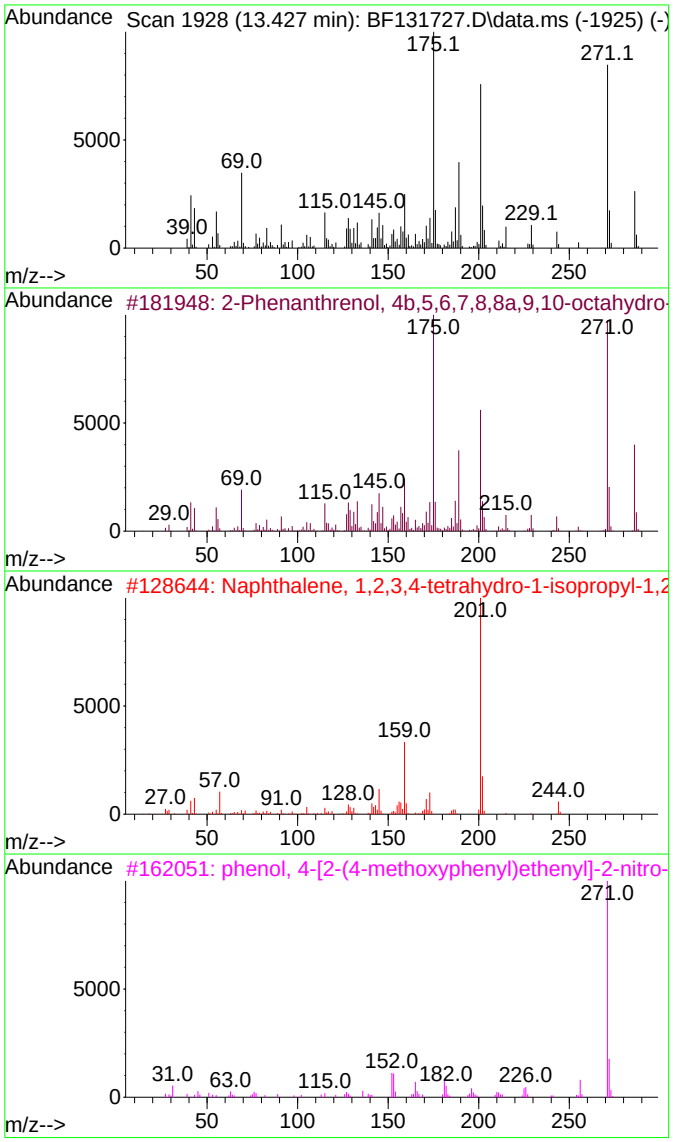
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

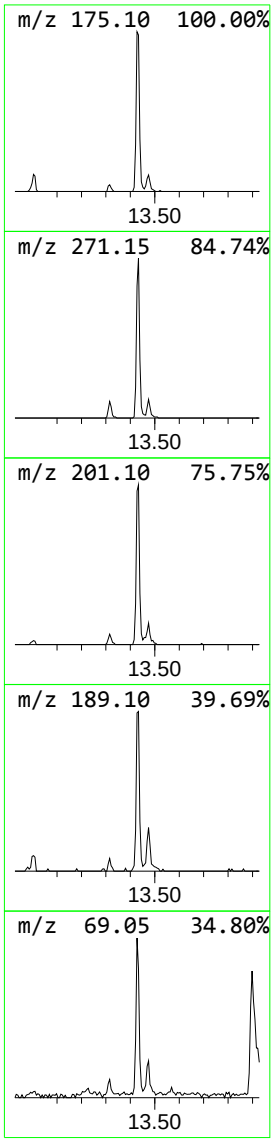
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.427	13.00 ng	294462	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	99
2	Naphthalene, 1,2,3,4-tetrahydro-...	244	C18H28	029577-17-1	20
3	phenol, 4-[2-(4-methoxyphenyl)et...	271	C15H13NO4	1000396-99-6	15
4	2,2-Bis(4'-methoxyphenyl)-2-etho...	286	C18H22O3	1000283-53-7	14
5	1H-naphtho[2,1-b]pyran-1-imine, ...	271	C19H13NO	1000401-75-2	11





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Sample : N6071-11
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FVSUB-TP8-COMP-08

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

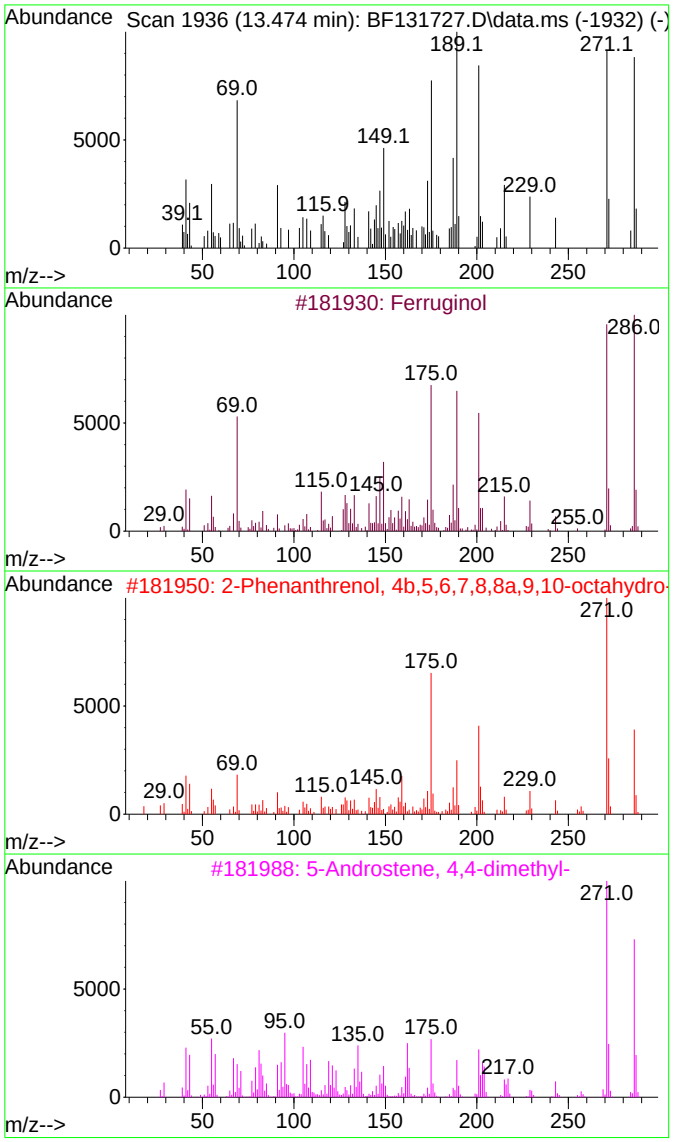
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

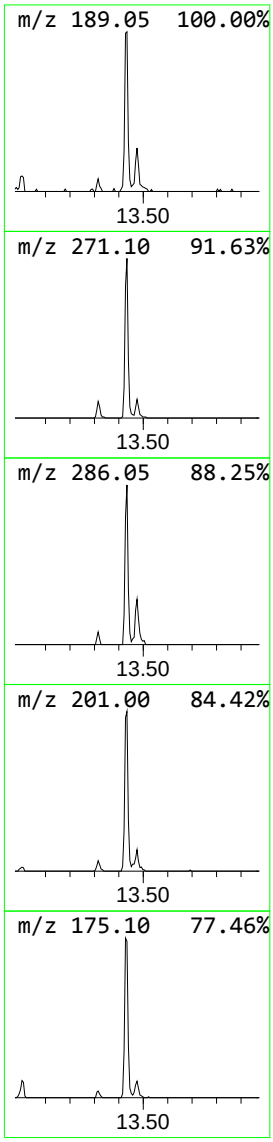
****

Peak Number 5 Ferruginol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.475	3.40 ng	77049	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ferruginol	286	C20H30O	000514-62-5	96
2	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	38
3	5-Androstene, 4,4-dimethyl-	286	C21H34	1000194-15-4	38
4	5.beta.-Pregn-11-ene	286	C21H34	006673-73-0	30
5	6,8-Difluoro-N-(4-methoxyphenyl)...	286	C16H12F2N2O	1000435-19-6	18





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FVSUB-TP8-COMP-08

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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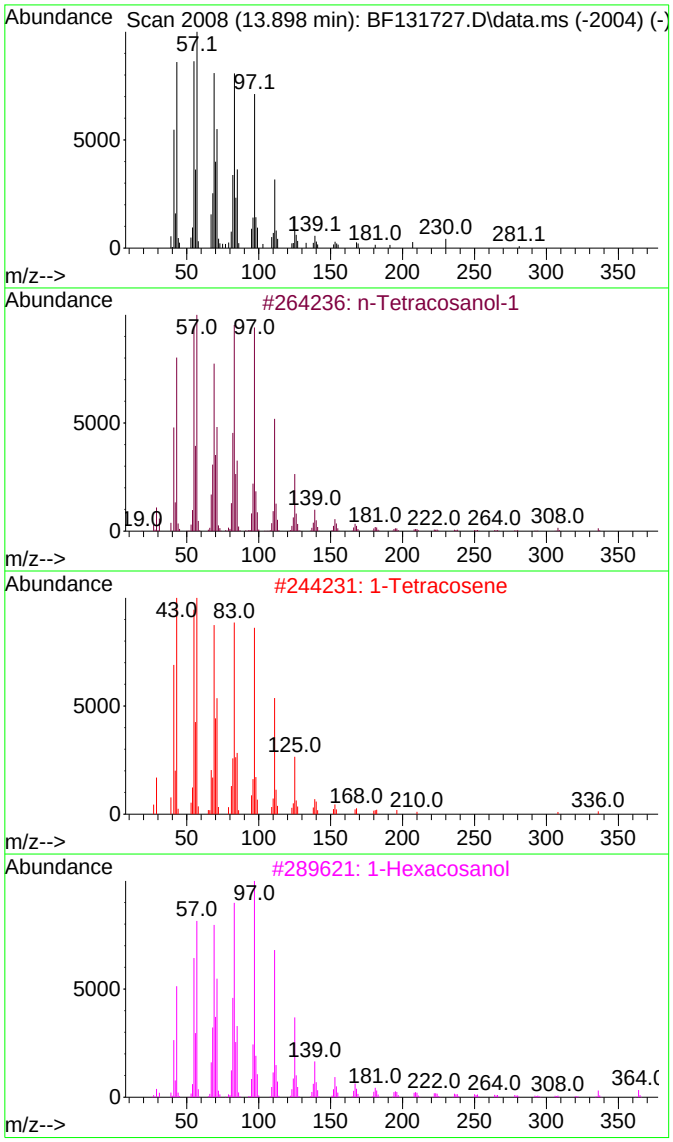
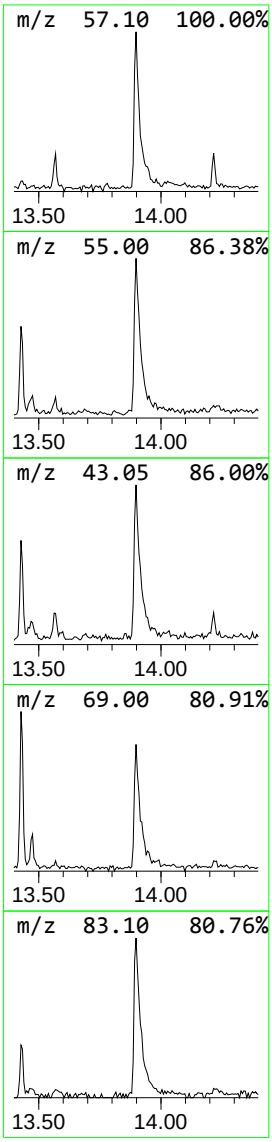
****

Peak Number 6 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	8.76 ng	198400	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	1-Tetracosene	336	C24H48	010192-32-2	91
3	1-Hexacosanol	382	C26H54O	000506-52-5	91
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
5	Behenic alcohol	326	C22H46O	000661-19-8	90





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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

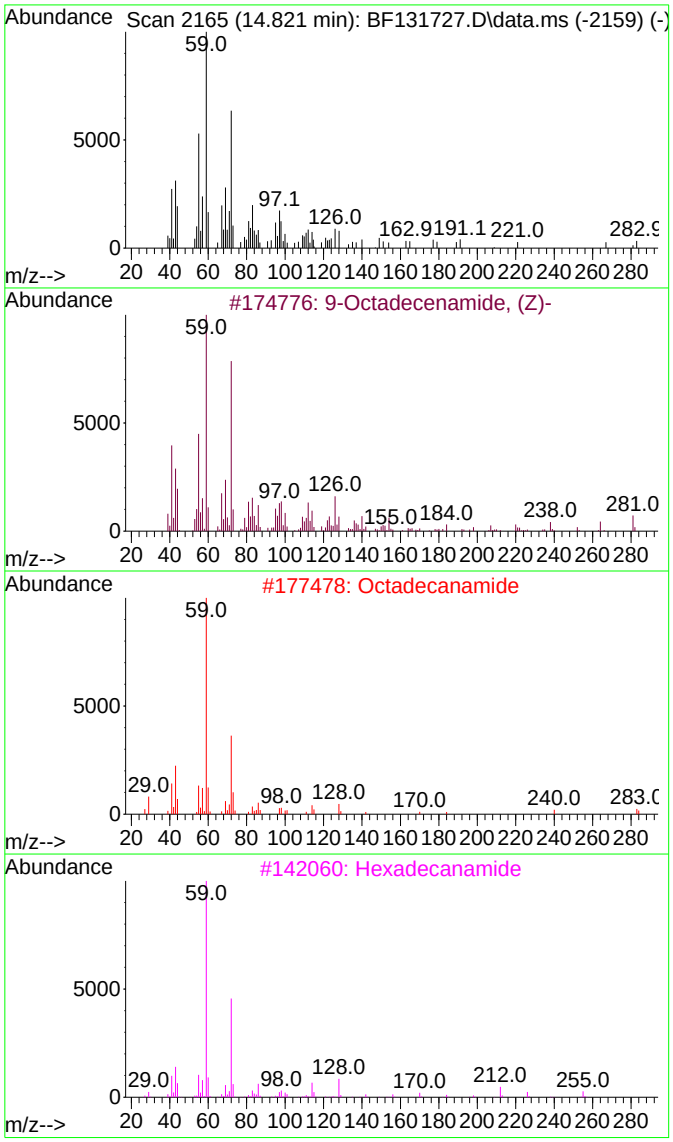
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

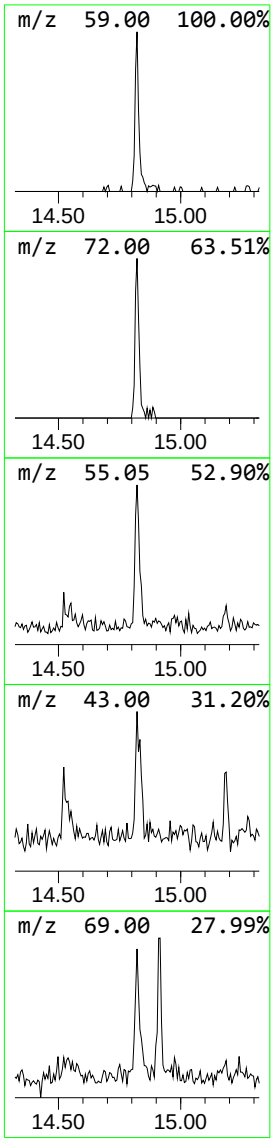
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	2.95 ng	62507	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	81
2	Octadecanamide	283	C18H37NO	000124-26-5	53
3	Hexadecanamide	255	C16H33NO	000629-54-9	53
4	Palmitoleamide	253	C16H31NO	106010-22-4	47
5	Tetradecanamide	227	C14H29NO	000638-58-4	43





Tentatively Identified Compound (LSC) summary

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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...	2.169	16.4	ng	392337	1	6.863	477233	20.0
2-Pentanone, 4-...	5.093	24.2	ng	577218	1	6.863	477233	20.0
Benzophenone	10.634	6.8	ng	250607	3	9.916	738808	20.0
2-Phenanthrenol...	13.427	13.0	ng	294462	5	14.057	453089	20.0
Ferruginol	13.475	3.4	ng	77049	5	14.057	453089	20.0
n-Tetracosanol-1	13.898	8.8	ng	198400	5	14.057	453089	20.0
9-Octadecenamid...	14.821	3.0	ng	62507	6	15.551	424010	20.0