LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
Data File : BF126566.D
Acq On : 10 Jan 2022 15:16
Operator : JU/CG
Sample : N1078-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEMP-WELL-1

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-BF122921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126566.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	488	492	500	rVB	83692	103451	3.42%	0.620%
2	5.386	557	561	564	rBV	2016487	1935534	63.97%	11.603%
3	6.404	729	734	737	rBV	1625613	1536209	50.77%	9.209%
4	6.769	792	796	799	rBV	650317	514373	17.00%	3.084%
5	7.333	886	892	895	rBV	1736132	1985066	65.61%	11.900%
6	7.957	995	998	1006	rBV	168104	154334	5.10%	0.925%
7	8.051	1010	1014	1017	rBV	849394	710131	23.47%	4.257%
8	9.133	1192	1198	1201	rBV	2959546	3025605	100.00%	18.138%
9	9.810	1308	1313	1316	rBV	855971	739255	24.43%	4.432%
10	10.227	1381	1384	1387	rBV2	36835	31138	1.03%	0.187%
11	10.598	1442	1447	1451	rBV	1728363	1826692	60.37%	10.950%
12	11.292	1561	1565	1569	rBV	751466	668626	22.10%	4.008%
13	11.833	1652	1657	1660	rBV	43177	50231	1.66%	0.301%
14	12.845	1825	1829	1832	rBV	30286	34446	1.14%	0.206%
15	12.886	1832	1836	1840	rVV	2112422	2271269	75.07%	13.616%
16	13.086	1866	1870	1874	rBV	97117	90690	3.00%	0.544%
17	13.798	1986	1991	1997	rBV4	35300	59683	1.97%	0.358%
18	13.939	2011	2015	2019	rBV	475668	416566	13.77%	2.497%
19	14.039	2026	2032	2037	rBV	74140	78383	2.59%	0.470%
20	15.392	2257	2262	2266	rBV	389743	449704	14.86%	2.696%

Sum of corrected areas: 16681386

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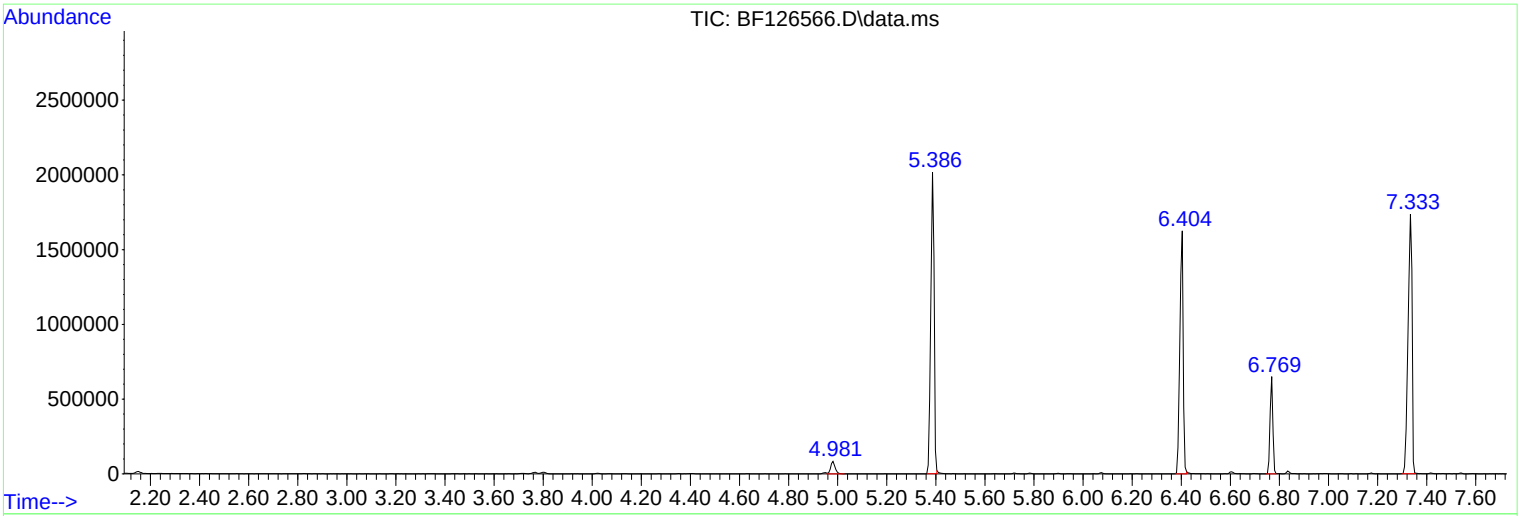
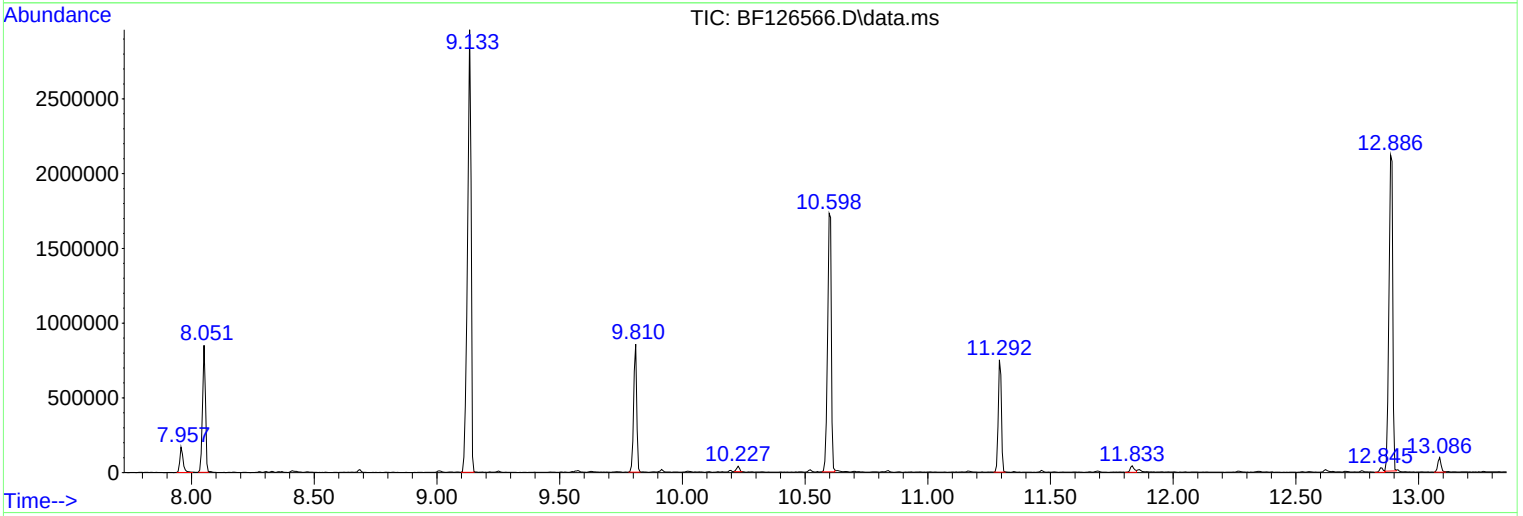
ALS Vial : 9 Sample Multiplier: 1

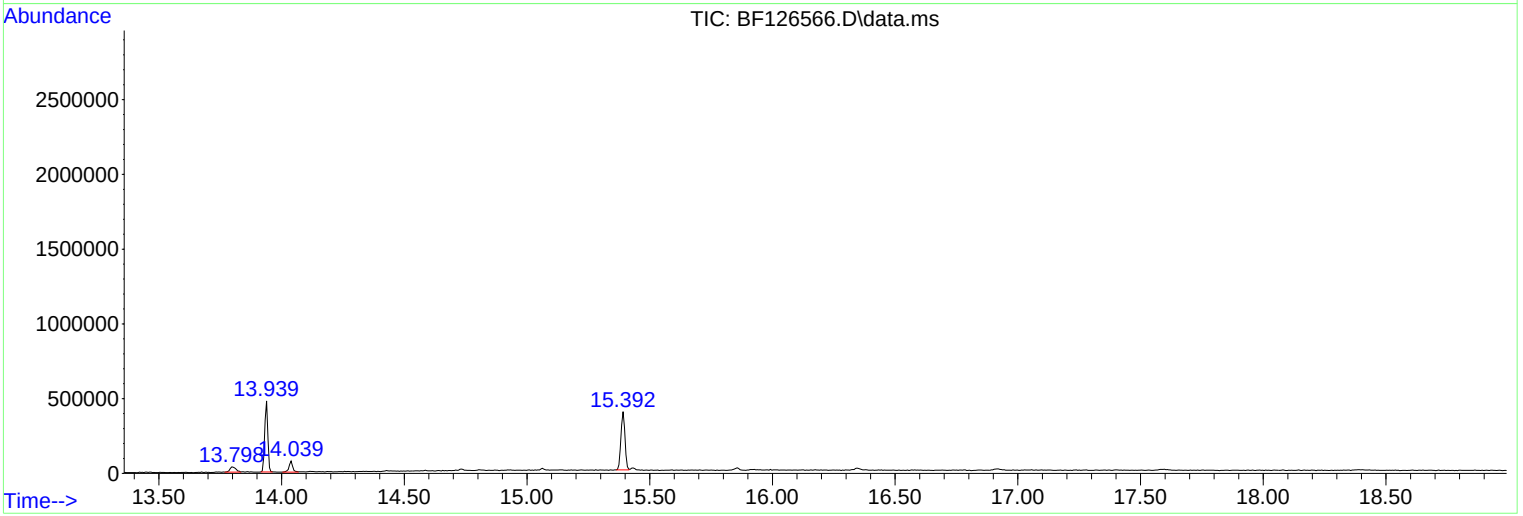
Instrument :
BNA_F
ClientSampleId :
TEMP-WELL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.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 : BF126566.D
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ClientSampleId :
TEMP-WELL-1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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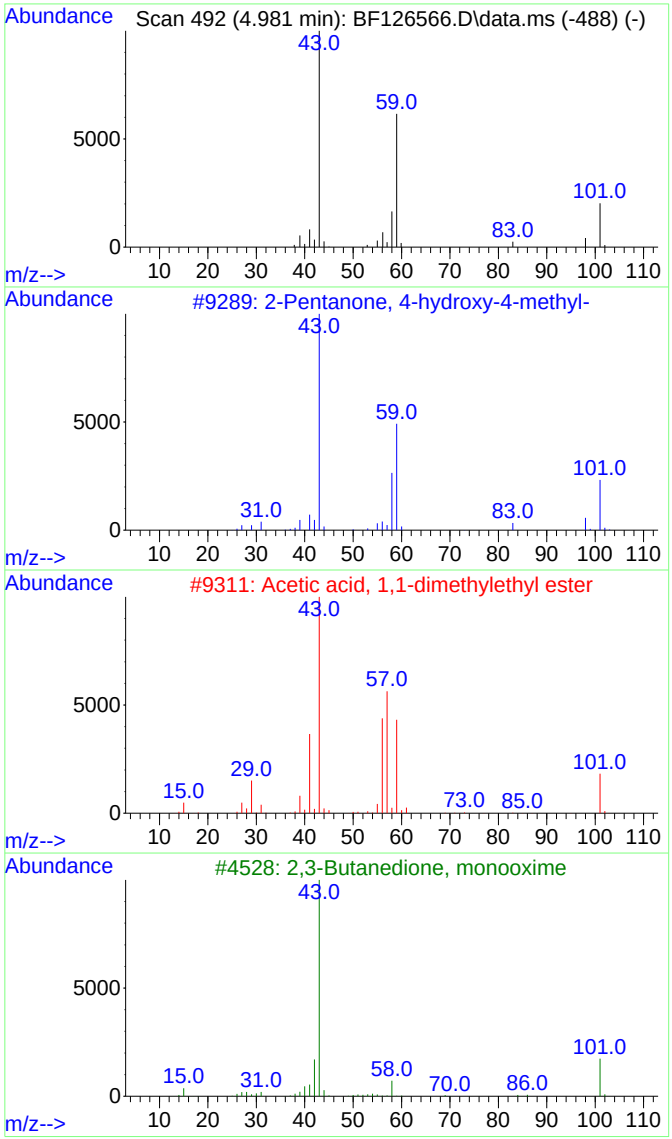
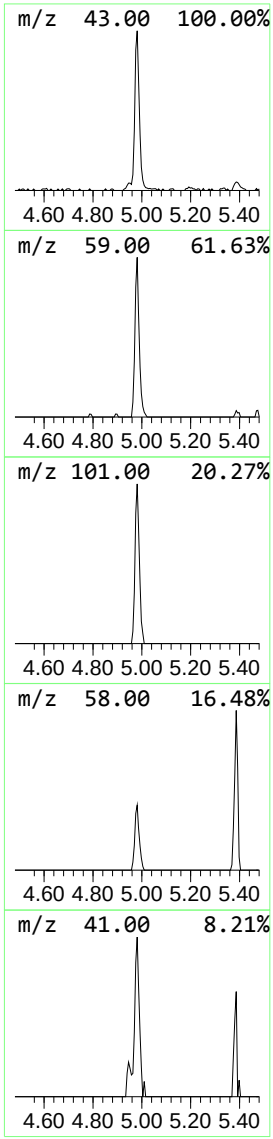
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	4.02 ng	103451	1,4-Dichlorobenzene-d4	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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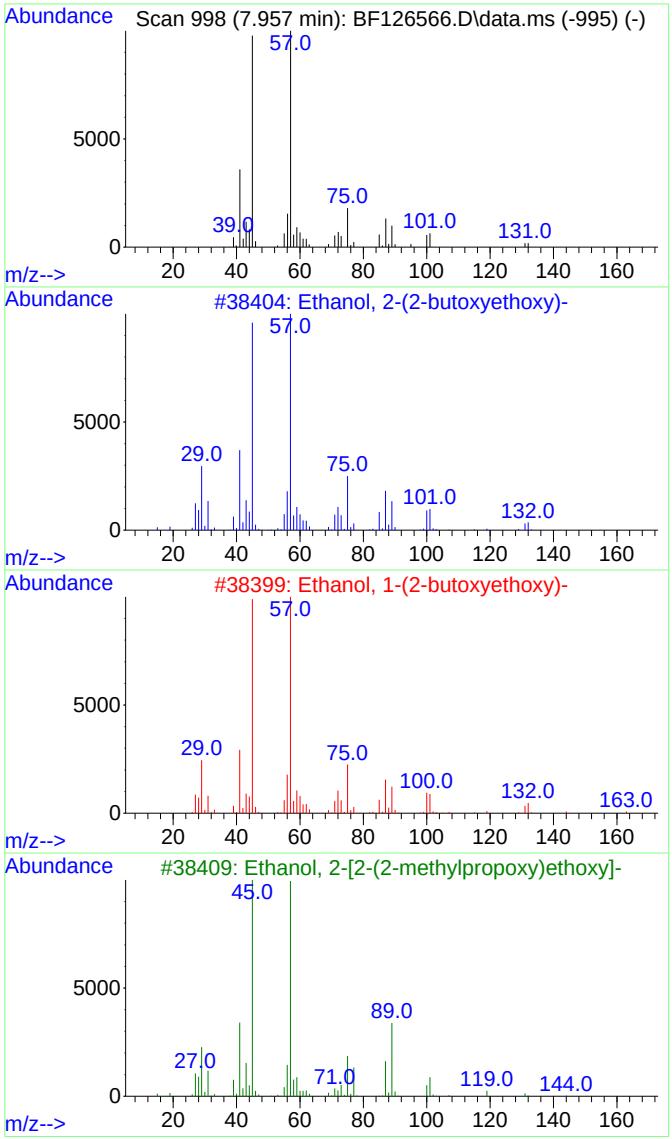
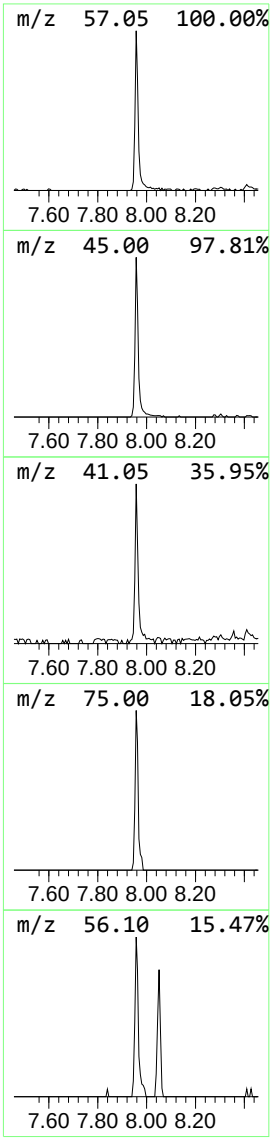
****

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.957	4.35 ng	154334	Naphthalene-d8	8.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
5	Hexane, 1-(methoxymethoxy)-	146	C8H18O2	066675-06-7	47





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Sample : N1078-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEMP-WELL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
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TIC Library : C:\Database\NIST20.L
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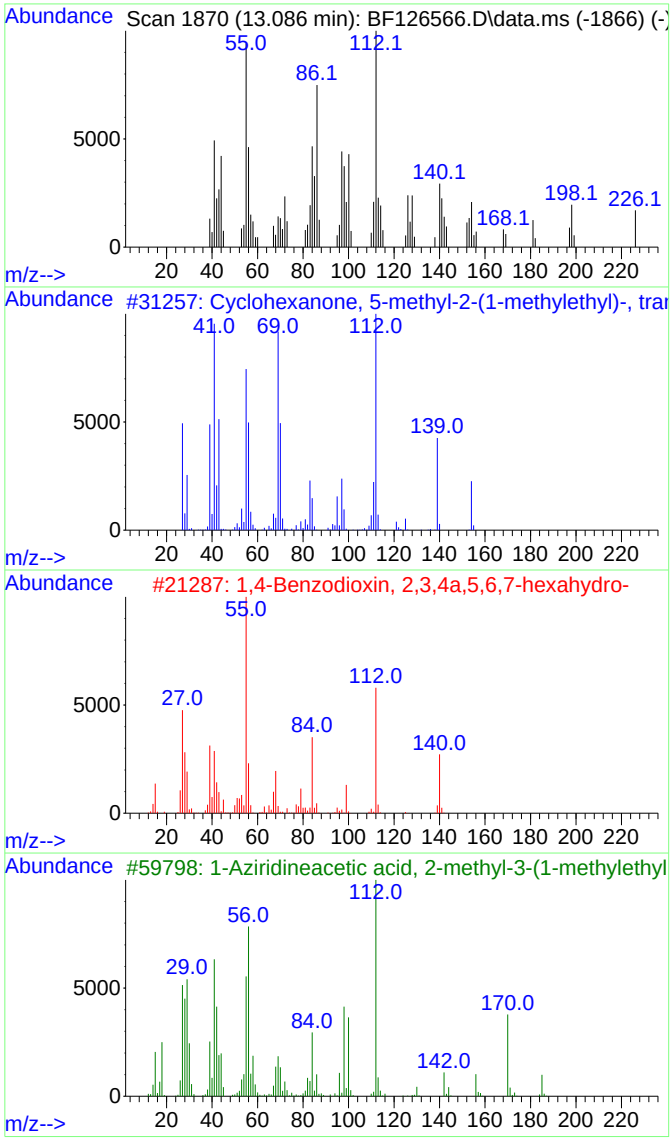
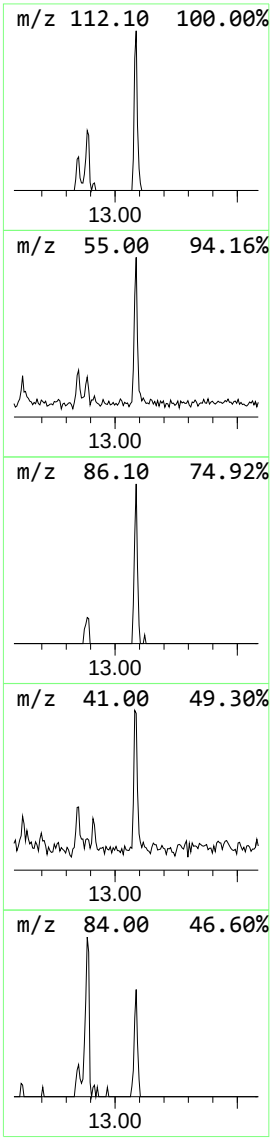
Peak Number 3 unknown13.086 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.086	4.35 ng	90690	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000089-80-5	25
2	1,4-Benzodioxin, 2,3,4a,5,6,7-he...	140	C8H12O2	055702-71-1	22
3	1-Aziridineacetic acid, 2-methyl...	185	C10H19NO2	055669-84-6	22
4	But-1-en-3-ynyl ethyl sulfide	112	C6H8S	1010298-90-7	22
5	Pivalaldehyde, semicarbazone	143	C6H13N3O	023809-33-8	18





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Operator : JU/CG
Sample : N1078-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEMP-WELL-1

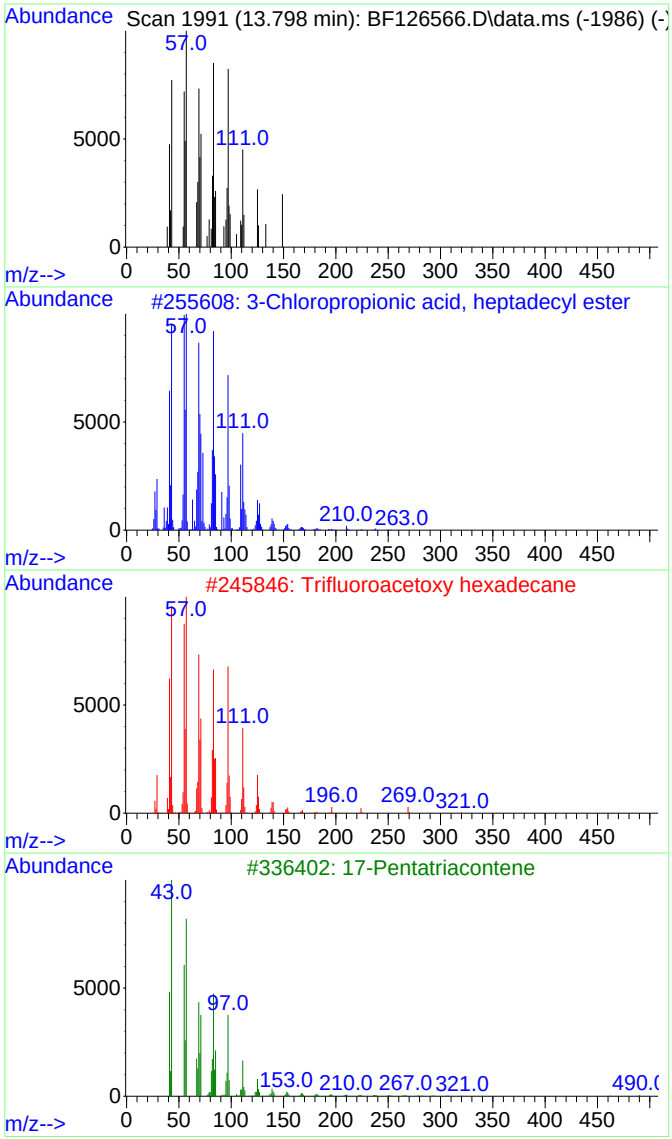
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

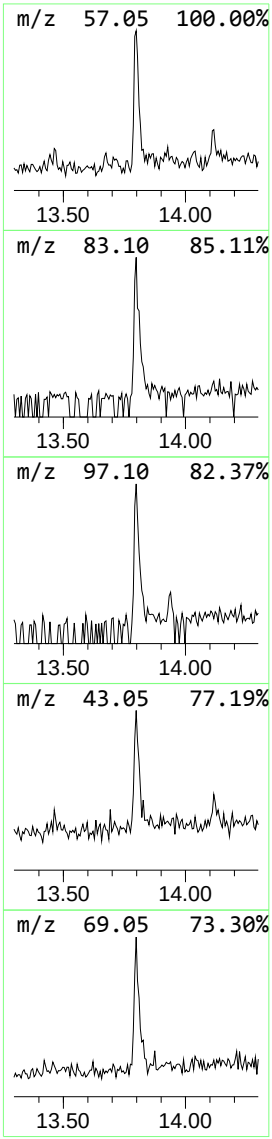
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Chloropropionic acid, hep... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.798	2.87 ng	59683	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	74
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	74
3	17-Pentatriacontene	491	C35H70	006971-40-0	72
4	11-Tricosene	322	C23H46	052078-56-5	64
5	1-Docosene	308	C22H44	001599-67-3	62





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Operator : JU/CG
Sample : N1078-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEMP-WELL-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

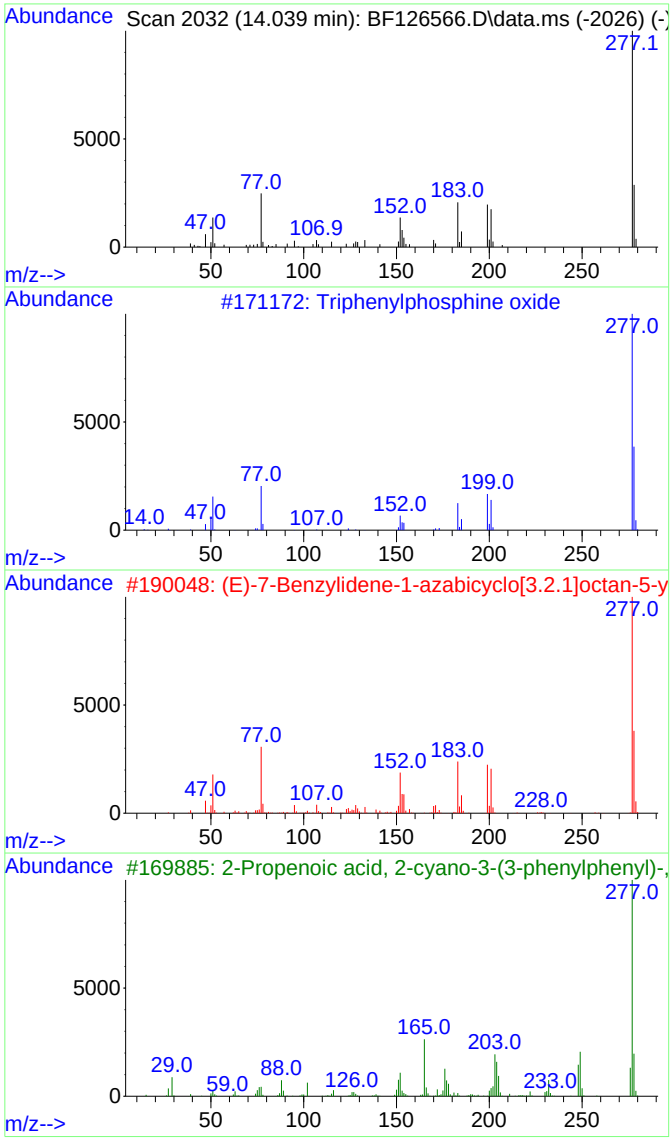
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

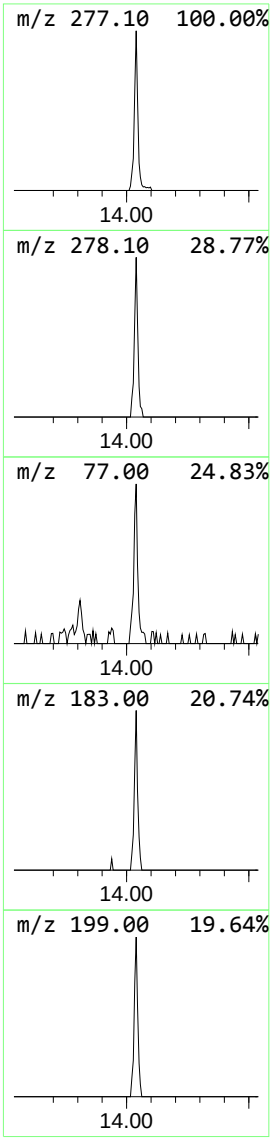
****

Peak Number 5 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.039	3.76 ng	78383	Chrysene-d12	13.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	2-Propenoic acid, 2-cyano-3-(3-p...	277	C18H15NO2	1000080-00-3	47
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
5	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	40





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011022\
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Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122921.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
2-Pentanone, 4-...	4.981	4.0	ng	103451	1	6.769	514373	20.0
Ethanol, 2-(2-b...	7.957	4.3	ng	154334	2	8.051	710131	20.0
unknown13.086	13.086	4.3	ng	90690	5	13.939	416566	20.0
3-Chloropropion...	13.798	2.9	ng	59683	5	13.939	416566	20.0
Triphenylphosph...	14.039	3.8	ng	78383	5	13.939	416566	20.0