LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121222\
Data File : BF131599.D
Acq On : 12 Dec 2022 18:39
Operator : CG\JU
Sample : N5976-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-SAMPLE-TANK-1-2-3-4-5

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-BF120822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131599.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	6	14	19	rVB	1359936	1738060	72.80%	13.374%
2	5.099	508	512	520	rVB	150676	171640	7.19%	1.321%
3	5.510	577	582	585	rBV	1156662	1071515	44.88%	8.245%
4	6.516	749	753	756	rBV	820926	707988	29.65%	5.448%
5	6.893	813	817	820	rBV	435194	372342	15.60%	2.865%
6	7.457	908	913	916	rBV	1233203	1297759	54.36%	9.986%
7	8.181	1031	1036	1039	rBV	549581	458123	19.19%	3.525%
8	8.875	1151	1154	1157	rBV	32953	31026	1.30%	0.239%
9	9.263	1214	1220	1223	rBV	2718840	2387536	100.00%	18.371%
10	9.945	1332	1336	1340	rBV	655137	528516	22.14%	4.067%
11	10.663	1455	1458	1461	rVB	116043	93498	3.92%	0.719%
12	10.739	1466	1471	1475	rBV	1503865	1437128	60.19%	11.058%
13	11.439	1586	1590	1594	rBV	589019	512810	21.48%	3.946%
14	11.969	1676	1680	1685	rBV	53133	53420	2.24%	0.411%
15	13.033	1857	1861	1865	rBV	1392522	1315687	55.11%	10.124%
16	13.998	2020	2025	2035	rBV6	34874	93338	3.91%	0.718%
17	14.098	2038	2042	2045	rVB	341478	318799	13.35%	2.453%
18	14.192	2053	2058	2063	rBV	57362	66287	2.78%	0.510%
19	15.610	2293	2299	2307	rBV	262106	340667	14.27%	2.621%

Sum of corrected areas: 12996139

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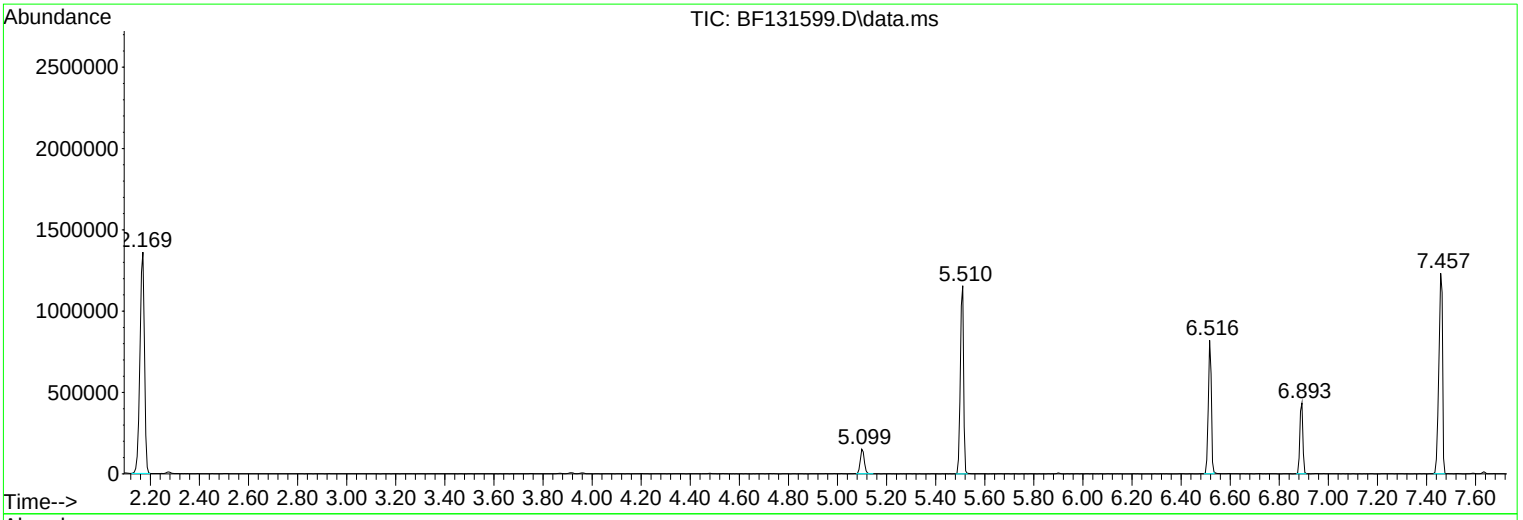
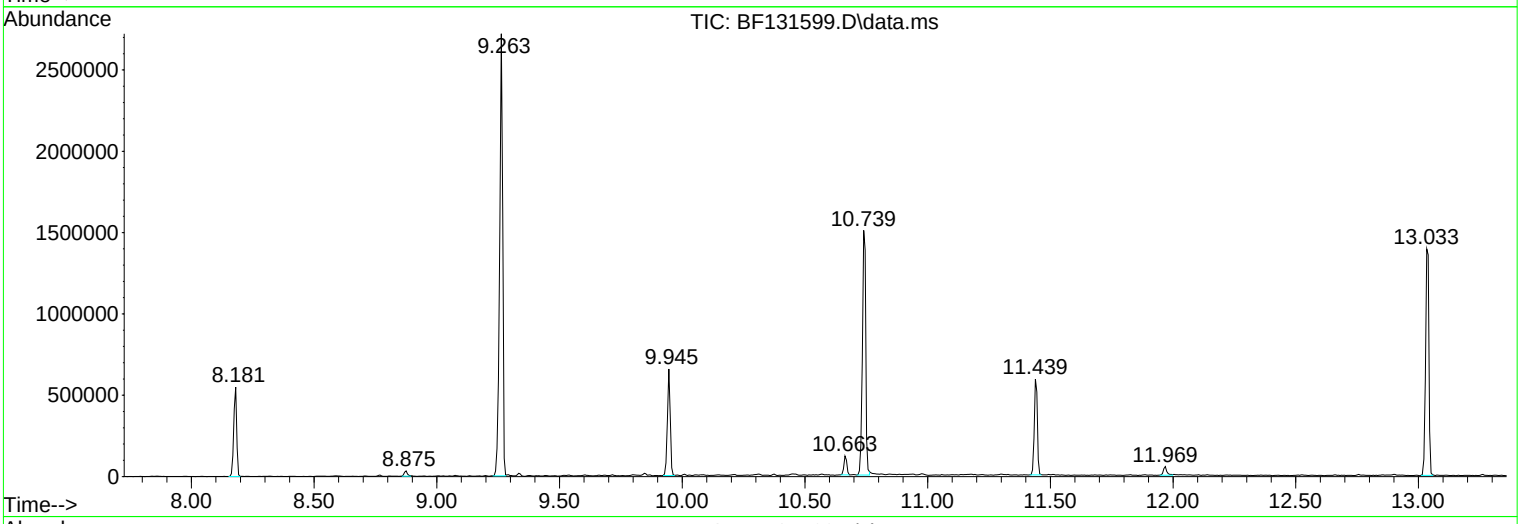
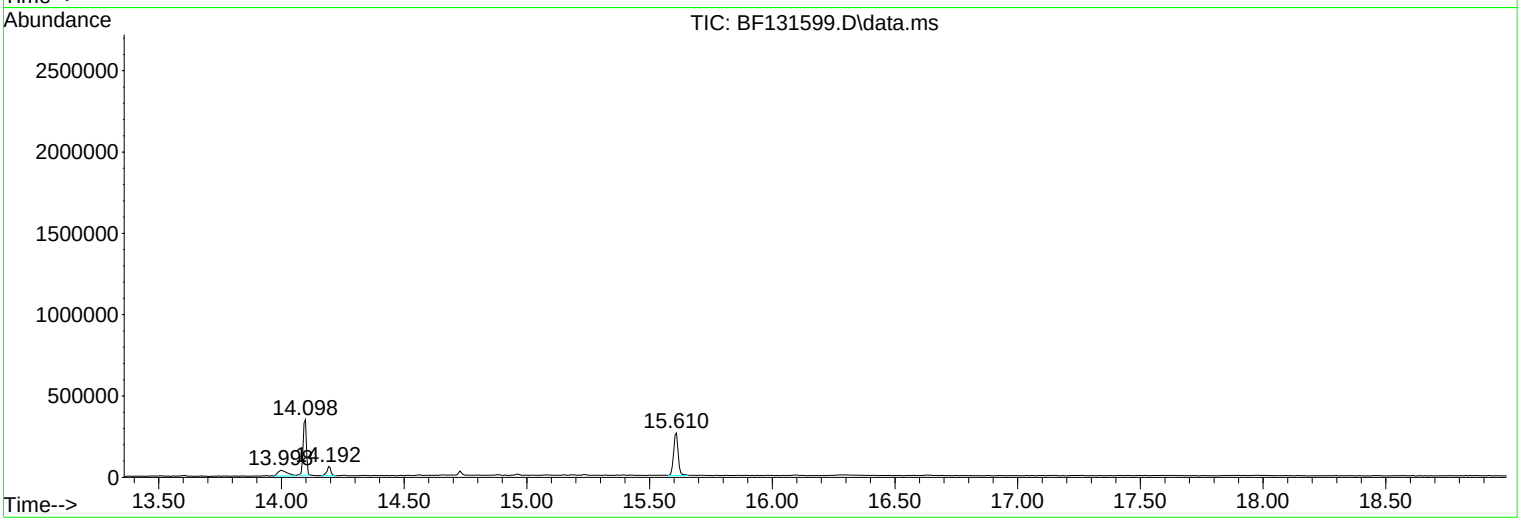
BNA_F
ClientSampleId :
COMP-SAMPLE-TANK-1-2-3-4-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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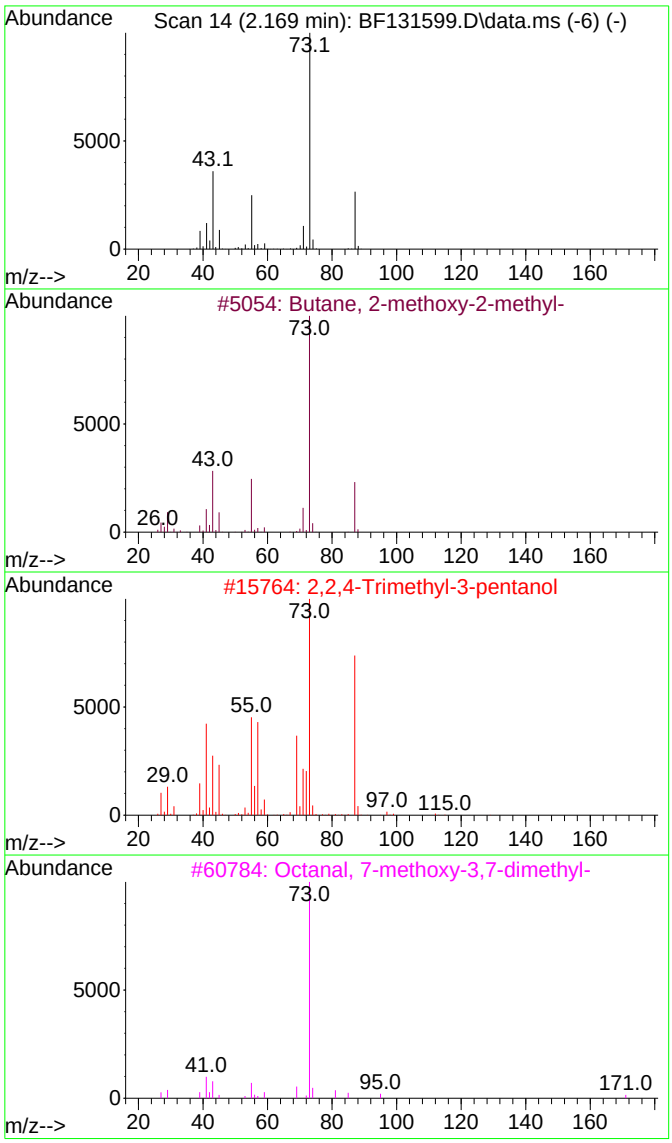
TIC Integration Parameters: LSCINT.P

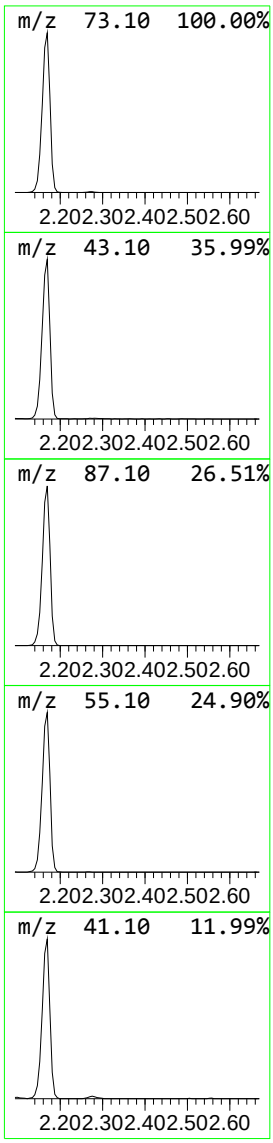
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	93.36 ng	1738060	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Sample : N5976-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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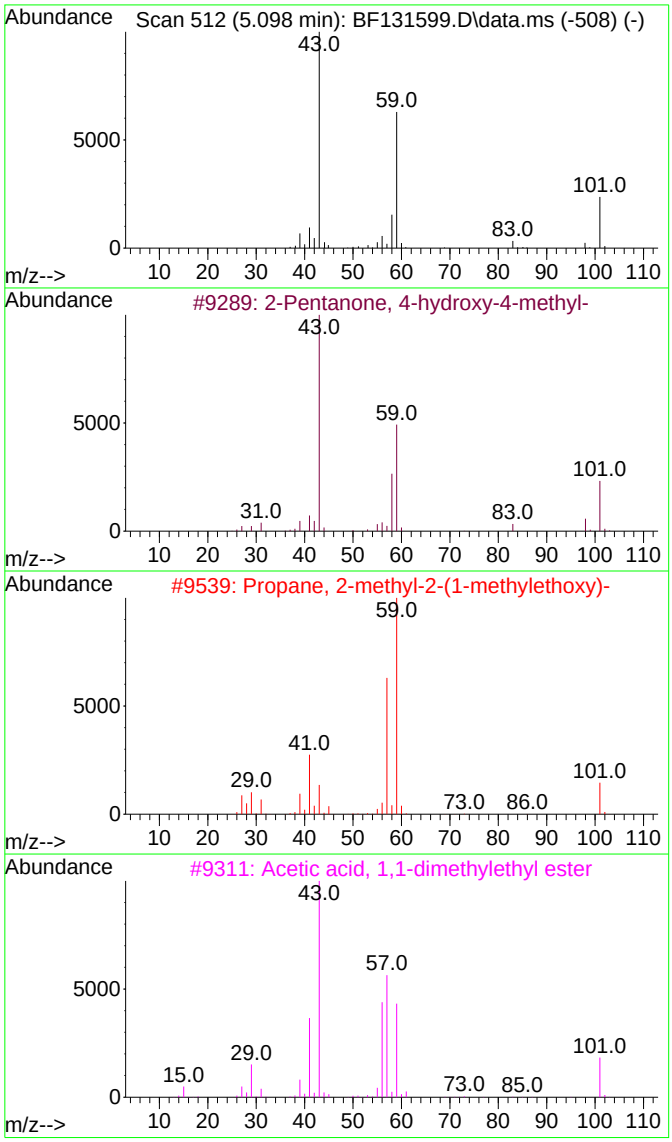
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

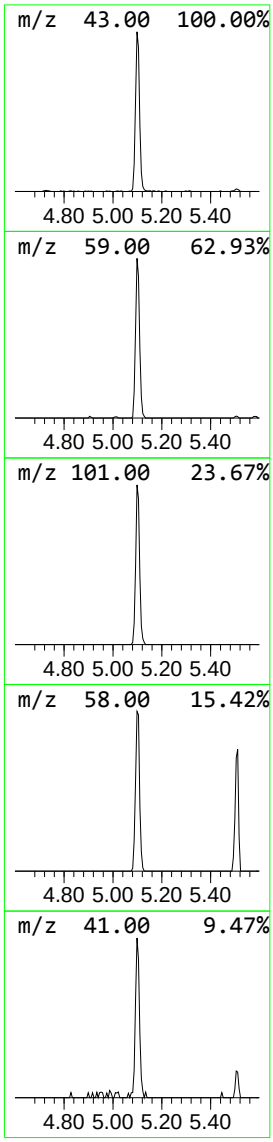
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	9.22 ng	171640	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28





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Data File : BF131599.D
Acq On : 12 Dec 2022 18:39
Operator : CG\JU
Sample : N5976-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-SAMPLE-TANK-1-2-3-4-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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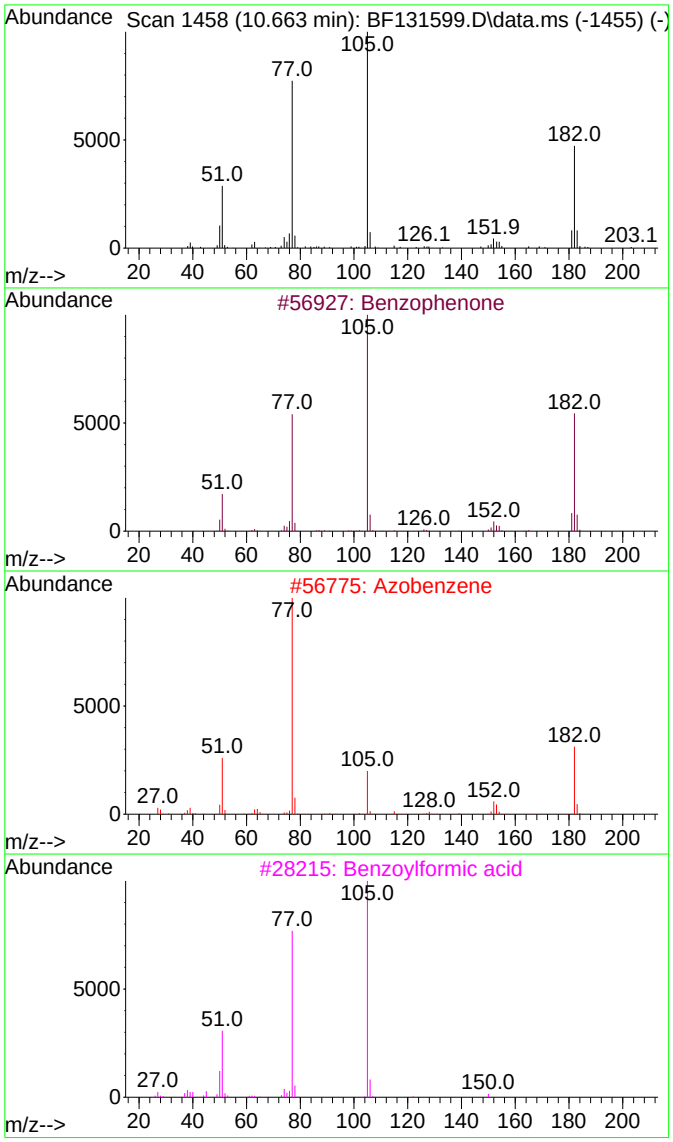
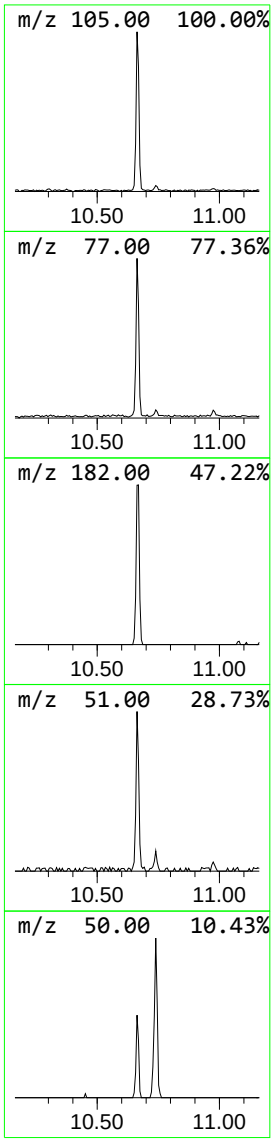
****

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.663	3.54 ng	93498	Acenaphthene-d10	9.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Azobenzene	182	C12H10N2	000103-33-3	72
3	Benzoylformic acid	150	C8H6O3	000611-73-4	70
4	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	58
5	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	53





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Data File : BF131599.D
Acq On : 12 Dec 2022 18:39
Operator : CG\JU
Sample : N5976-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
COMP-SAMPLE-TANK-1-2-3-4-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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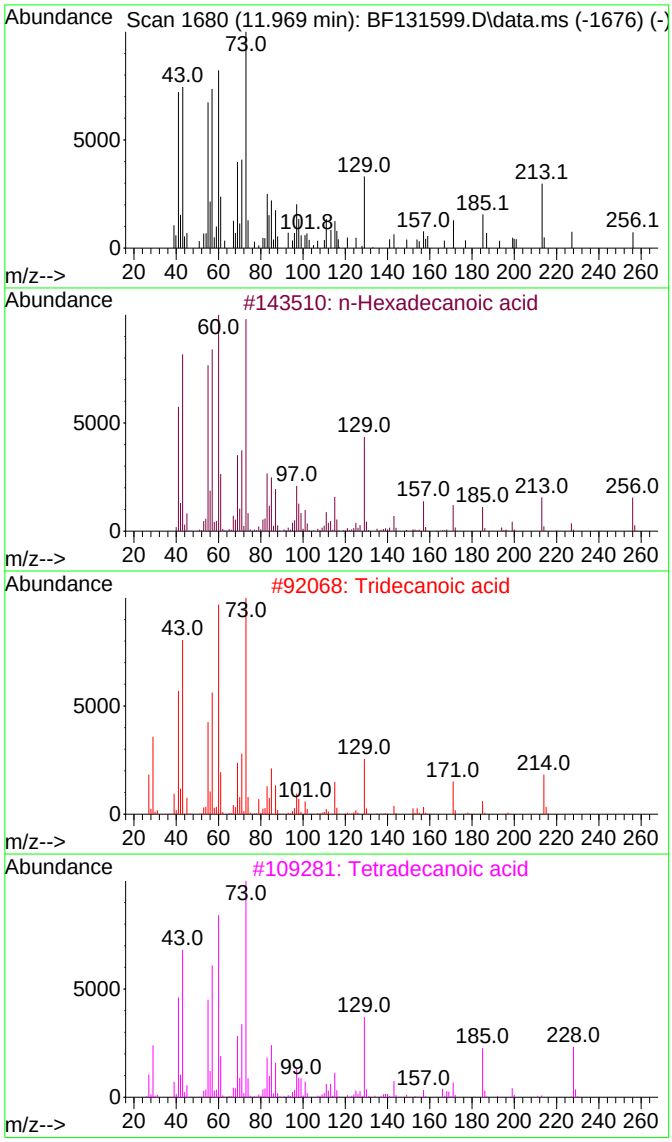
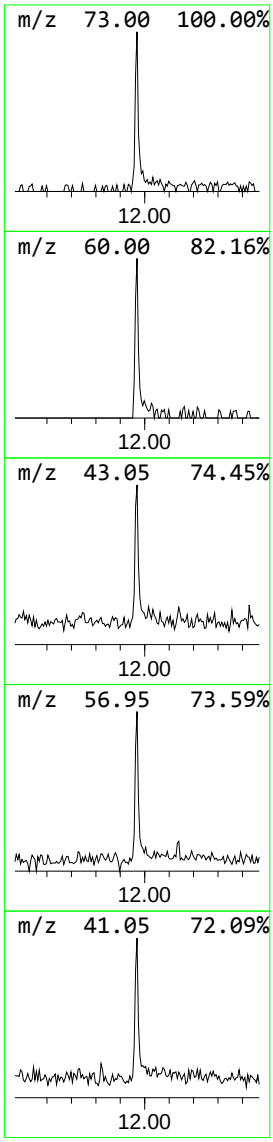
Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	2.08 ng	53420	Phenanthrene-d10	11.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Dodecanoic acid	200	C12H24O2	000143-07-7	68
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	50





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BNA_F
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COMP-SAMPLE-TANK-1-2-3-4-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

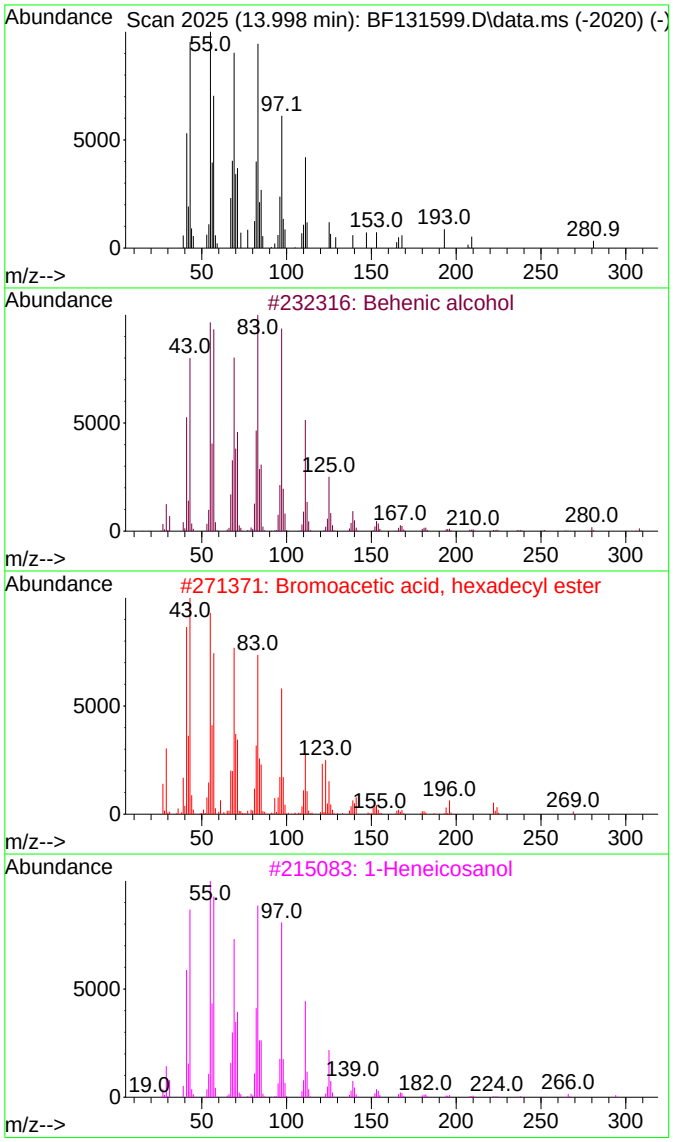
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

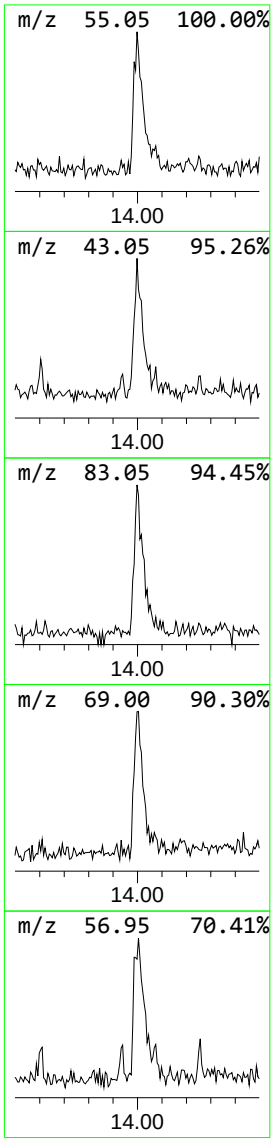
****

Peak Number 5 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	5.86 ng	93338	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	76
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	70
3	1-Heneicosanol	312	C21H44O	015594-90-8	68
4	1-Tetracosene	336	C24H48	010192-32-2	62
5	1-Eicosanol	298	C20H42O	000629-96-9	60





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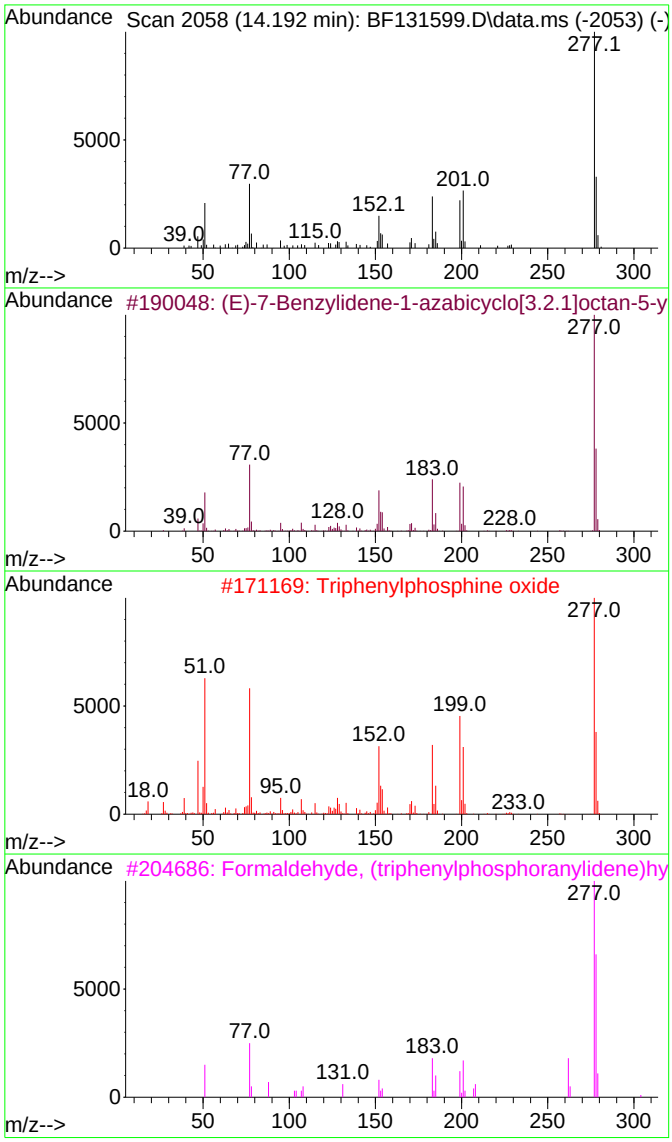
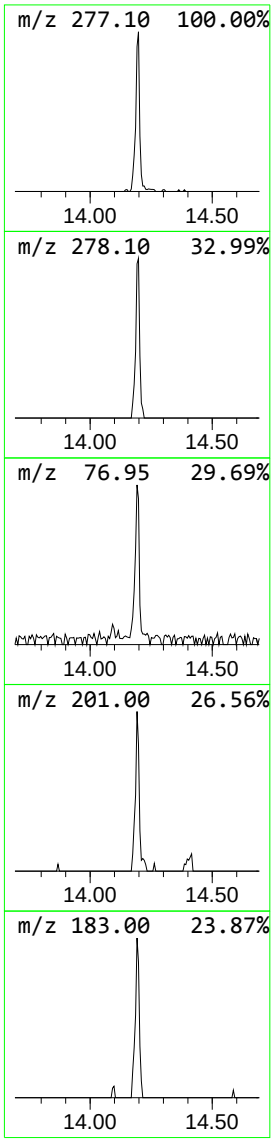
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (E)-7-Benzylidene-1-azabicy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	4.16 ng	66287	Chrysene-d12	14.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	87
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	83
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4	Furo[3,2-c]quinoline, 8-bromo-2,...	277	C13H12BrNO	1000310-92-7	43
5	2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	38





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.169	93.4	ng	1738060	1	6.893	372342	20.0
2-Pentanone, 4-...	5.098	9.2	ng	171640	1	6.893	372342	20.0
Benzophenone	10.663	3.5	ng	93498	3	9.945	528516	20.0
n-Hexadecanoic ...	11.969	2.1	ng	53420	4	11.439	512810	20.0
Behenic alcohol	13.998	5.9	ng	93338	5	14.098	318799	20.0
(E)-7-Benzylide...	14.192	4.2	ng	66287	5	14.098	318799	20.0