LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
Data File : BF140130.D
Acq On : 29 Oct 2024 23:24
Operator : RC/JU
Sample : P4597-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BLUE-2-2

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-BF101824.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140130.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	9	17	24	rVB	824940	1314550	47.39%	6.625%
2	4.504	404	410	419	rBV	125955	183568	6.62%	0.925%
3	5.116	505	514	523	rBV	331567	511075	18.42%	2.576%
4	5.375	553	558	566	rVB	41285	56045	2.02%	0.282%
5	5.510	575	581	586	rBV	1747866	2304894	83.08%	11.617%
6	5.904	643	648	655	rVB	75173	94682	3.41%	0.477%
7	6.510	744	751	756	rBV	1696174	2310561	83.29%	11.646%
8	6.887	810	815	821	rVB	627171	773906	27.90%	3.901%
9	7.445	904	910	915	rBV	1225889	1607384	57.94%	8.101%
10	8.169	1027	1033	1038	rBV	801460	994052	35.83%	5.010%
11	9.245	1210	1216	1225	rBV	2089741	2774152	100.00%	13.982%
12	9.922	1326	1331	1346	rVB	808757	1026570	37.00%	5.174%
13	10.634	1446	1452	1460	rBV	126940	162204	5.85%	0.818%
14	10.710	1460	1465	1481	rBV	971401	1233015	44.45%	6.215%
15	10.945	1501	1505	1512	rVB	32848	40072	1.44%	0.202%
16	11.410	1579	1584	1591	rBV	648357	798547	28.79%	4.025%
17	11.933	1668	1673	1696	rBV2	136738	246804	8.90%	1.244%
18	12.716	1800	1806	1819	rBV4	27571	66128	2.38%	0.333%
19	12.998	1848	1854	1859	rBV	1472640	1883673	67.90%	9.494%
20	13.898	2001	2007	2025	rBV	48246	135157	4.87%	0.681%
21	14.051	2028	2033	2039	rBV	532983	689724	24.86%	3.476%
22	15.539	2280	2286	2300	rVV	379969	634027	22.85%	3.196%

Sum of corrected areas: 19840790

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102924\
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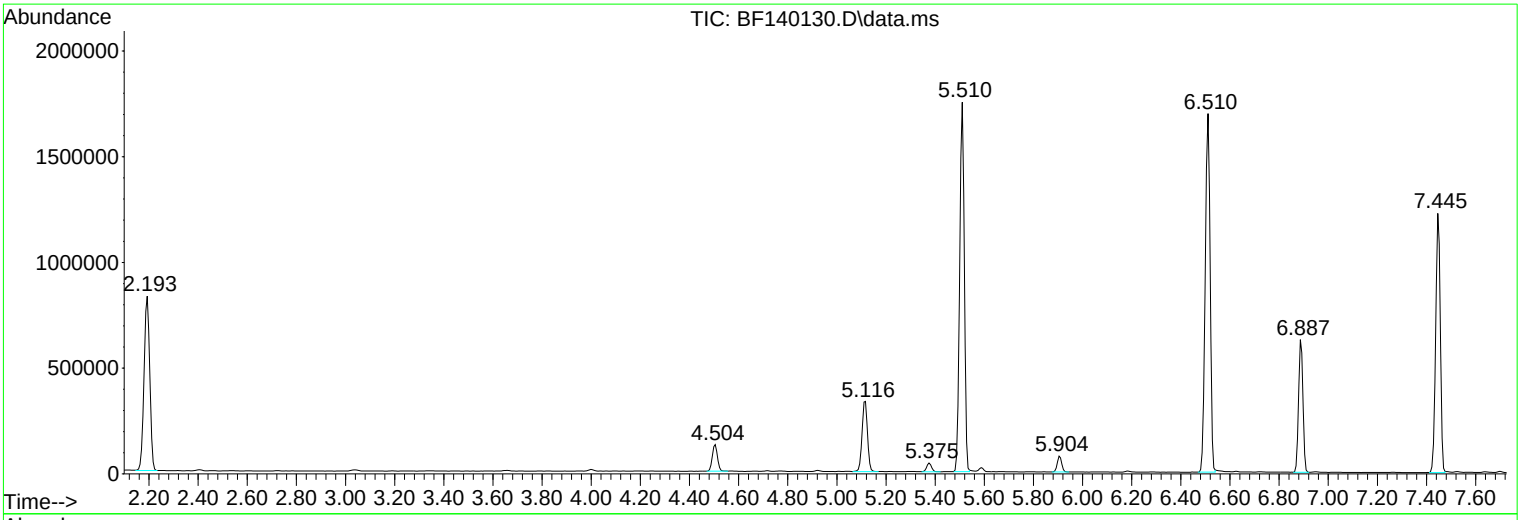
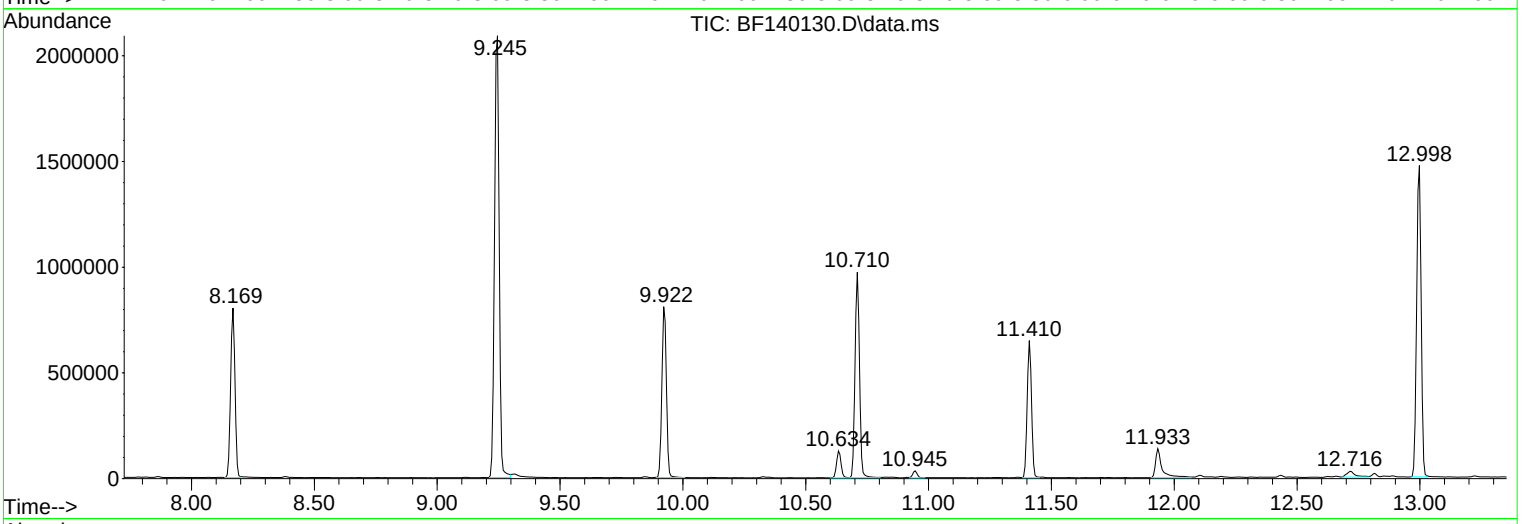
Sample : P4597-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

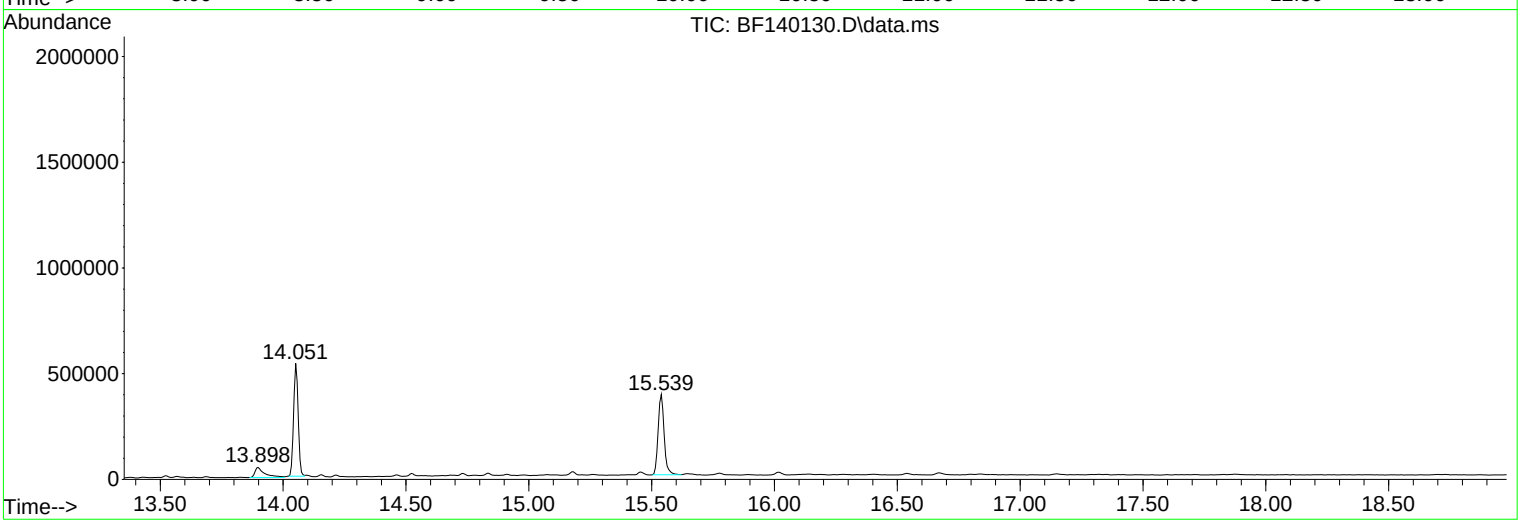
Instrument :
BNA_F
ClientSampleId :
BLUE-2-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.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 : BF140130.D
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Operator : RC/JU
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

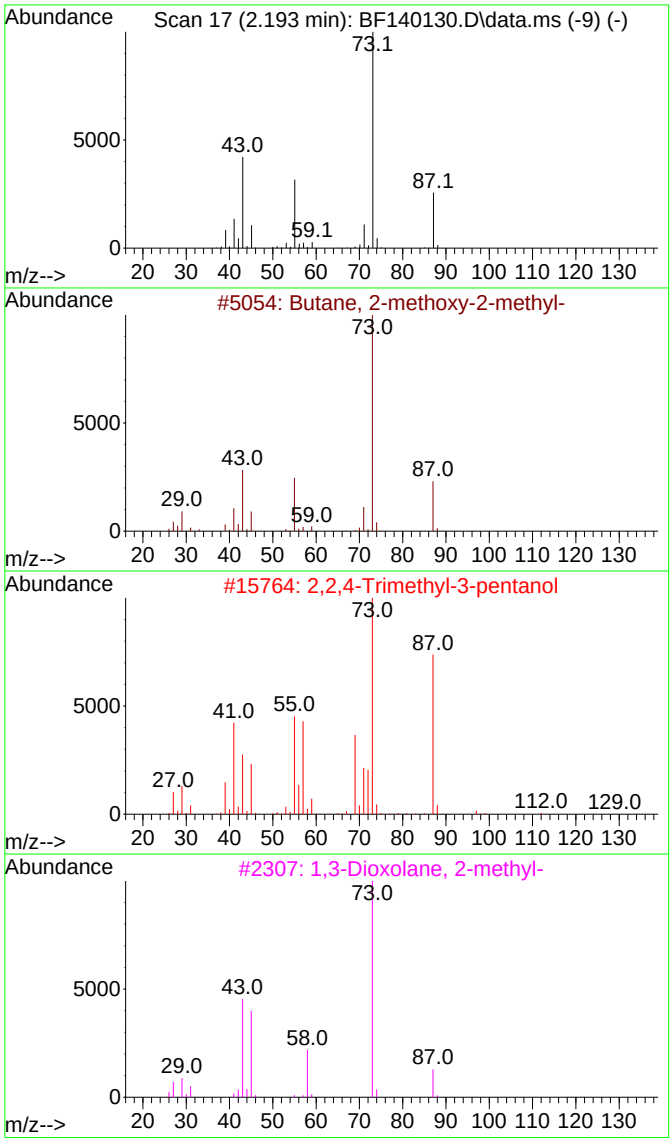
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

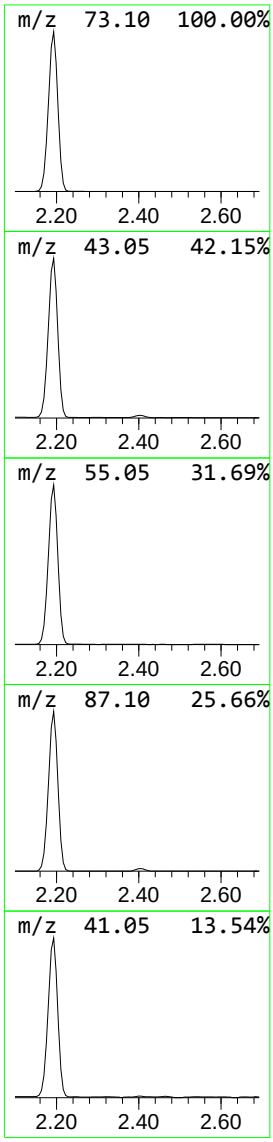
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	33.97 ng	1314550	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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Data File : BF140130.D
Acq On : 29 Oct 2024 23:24
Operator : RC/JU
Sample : P4597-10
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Instrument :
BNA_F
ClientSampleId :
BLUE-2-2

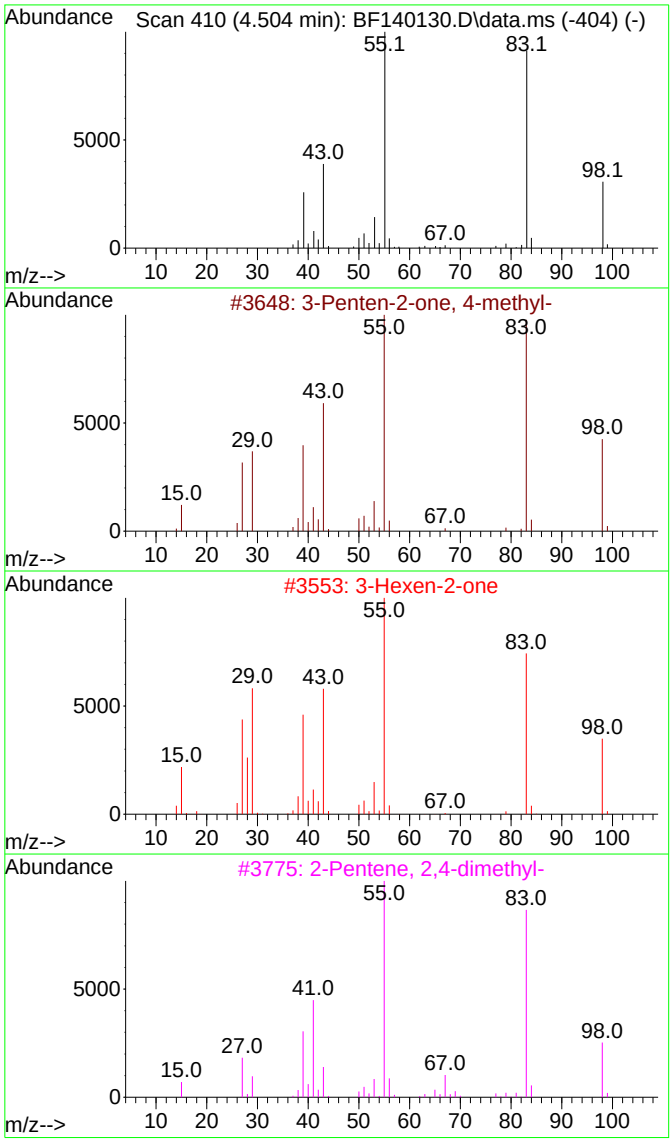
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

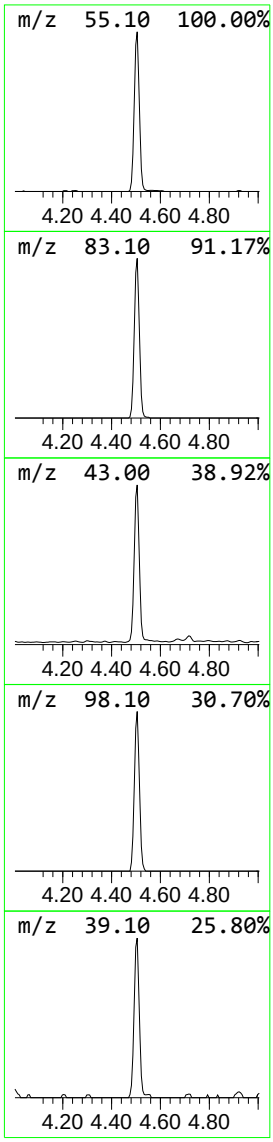
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.504	4.74 ng	183568	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	78





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Data File : BF140130.D
Acq On : 29 Oct 2024 23:24
Operator : RC/JU
Sample : P4597-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BLUE-2-2

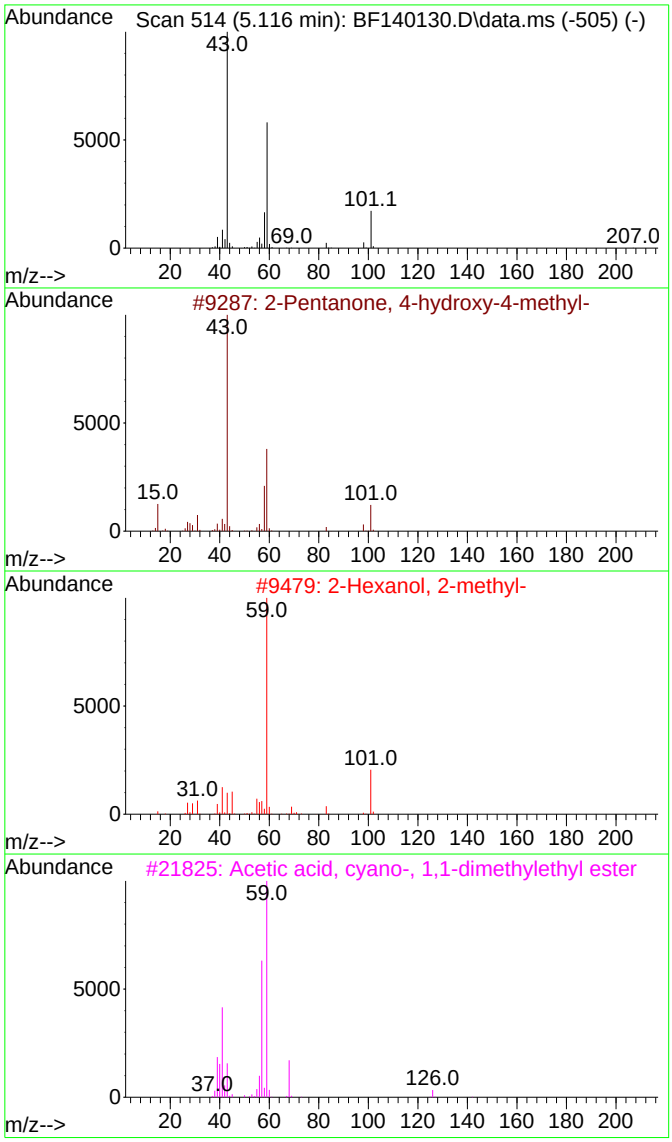
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

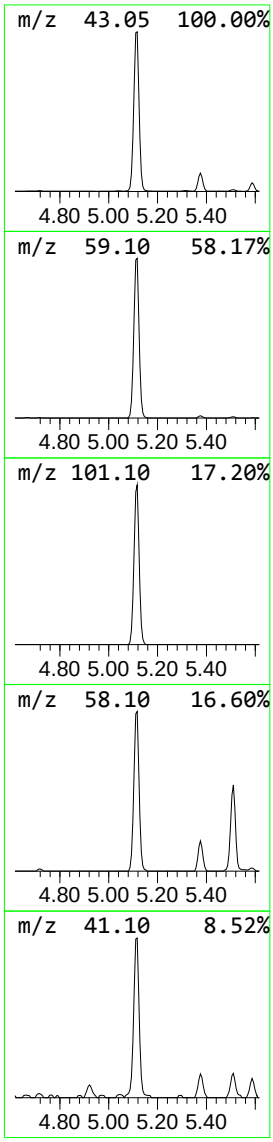
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	13.21 ng	511075	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	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Guanidine	59	CH5N3	000113-00-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Data File : BF140130.D
Acq On : 29 Oct 2024 23:24
Operator : RC/JU
Sample : P4597-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BLUE-2-2

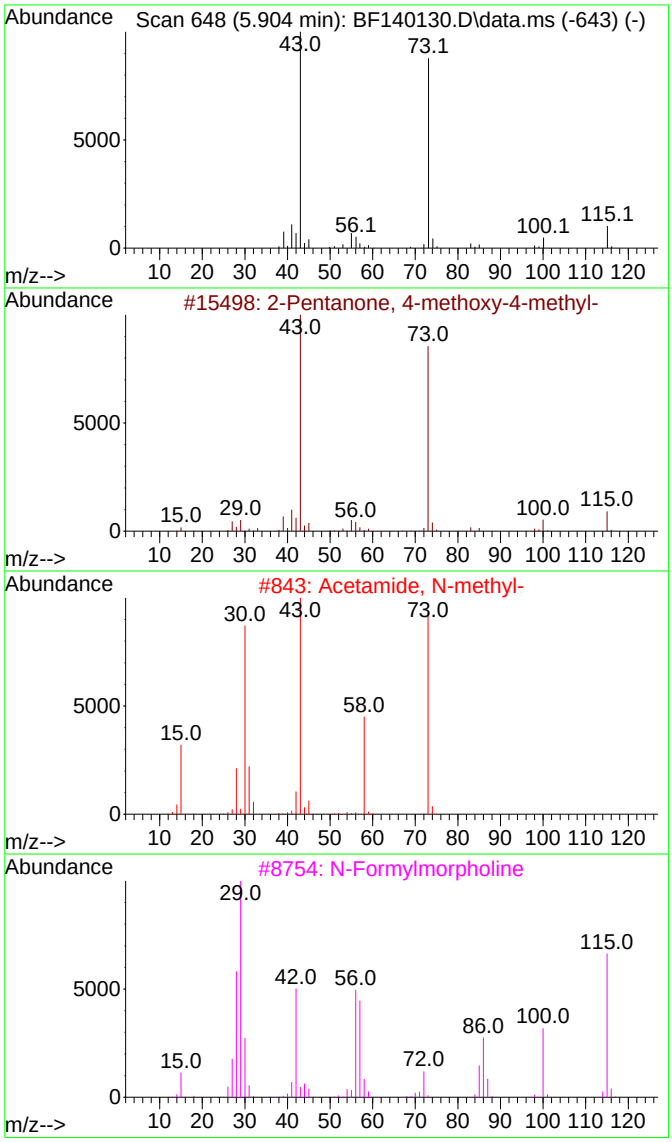
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

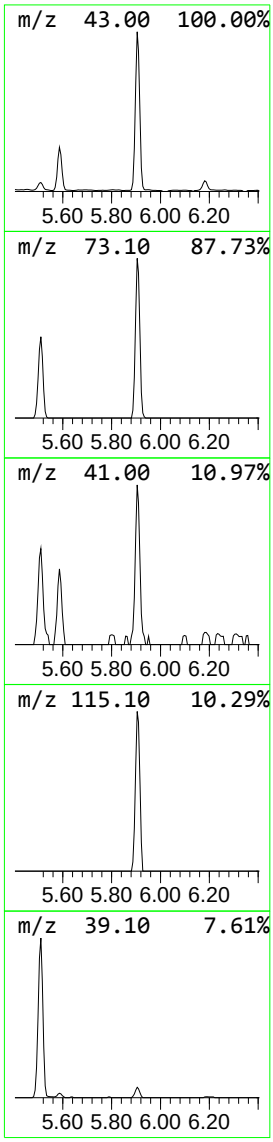
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.904	2.45 ng	94682	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
3	N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
4	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





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Operator : RC/JU
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BLUE-2-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

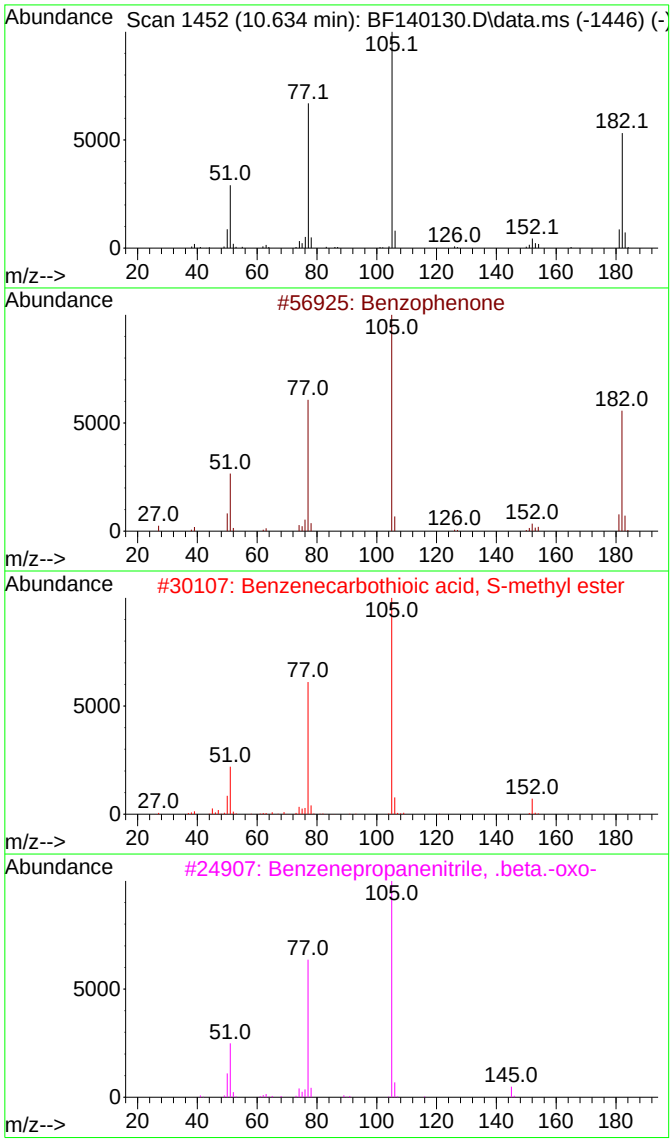
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

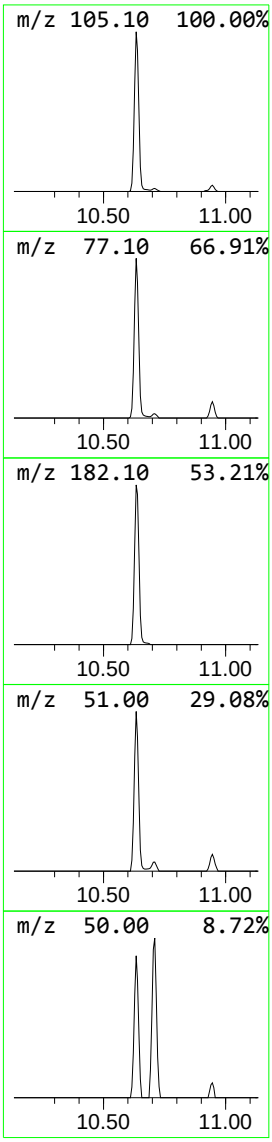
****

Peak Number 5 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.634	3.16 ng	162204	Acenaphthene-d10	9.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	64
3	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	49
4	Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47
5	2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47





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Sample : P4597-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BLUE-2-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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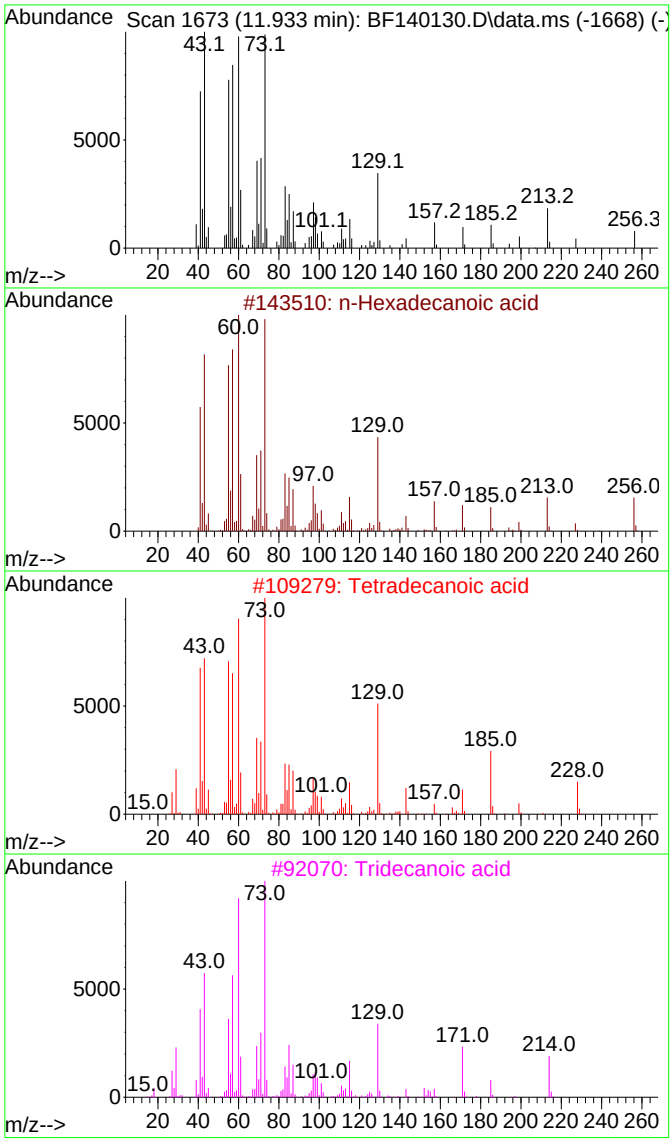
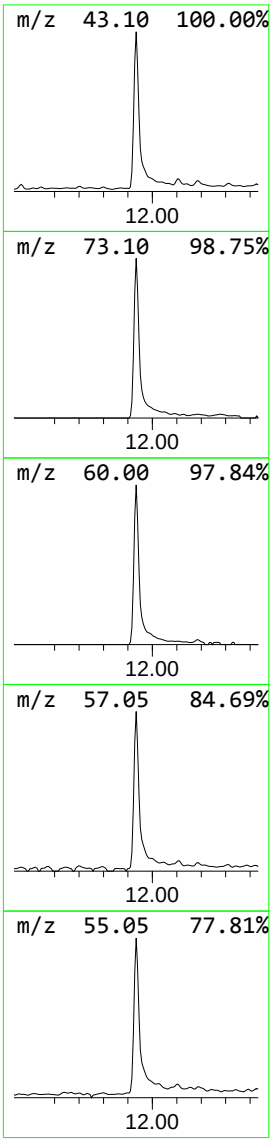
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	6.18 ng	246804	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5	Undecanoic acid	186	C11H22O2	000112-37-8	68





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Acq On : 29 Oct 2024 23:24
Operator : RC/JU
Sample : P4597-10
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BLUE-2-2

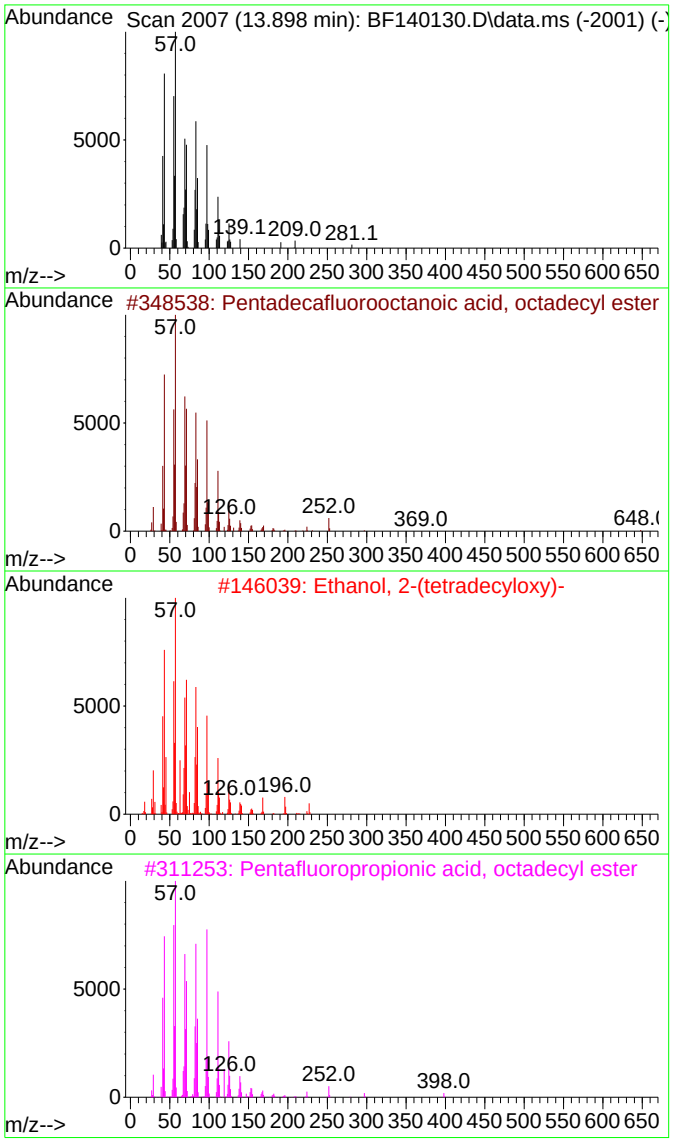
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101824.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

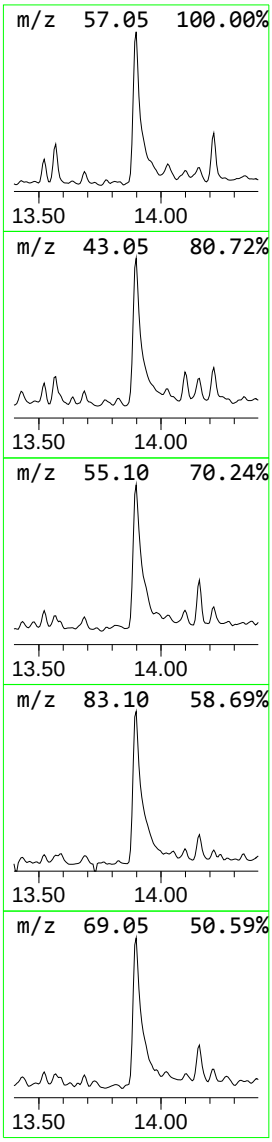
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	3.92 ng	135157	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
4	1-Hexacosanol	382	C26H54O	000506-52-5	91
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91





Tentatively Identified Compound (LSC) summary

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Data File : BF140130.D
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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...	2.193	34.0	ng	1314550	1	6.887	773906	20.0
3-Penten-2-one,...	4.504	4.7	ng	183568	1	6.887	773906	20.0
2-Pentanone, 4-...	5.116	13.2	ng	511075	1	6.887	773906	20.0
2-Pentanone, 4-...	5.904	2.5	ng	94682	1	6.887	773906	20.0
Benzophenone	10.634	3.2	ng	162204	3	9.922	1026570	20.0
n-Hexadecanoic ...	11.933	6.2	ng	246804	4	11.410	798547	20.0
Pentadecafluoro...	13.898	3.9	ng	135157	5	14.051	689724	20.0