LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133106.D
Acq On : 27 Apr 2023 18:25
Operator : CG\JU
Sample : 02502-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-511-COMP-02

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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133106.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.293	368	375	381	rBV	129395	164359	2.74%	0.394%
2	4.940	479	485	495	rVB	1092966	1522861	25.36%	3.652%
3	5.357	550	556	559	rBV	4747032	4831857	80.47%	11.587%
4	5.745	619	622	626	rBV	78635	67038	1.12%	0.161%
5	6.375	723	729	732	rBV	4189568	5100241	84.94%	12.231%
6	6.734	786	790	793	rBV	1534615	1170420	19.49%	2.807%
7	7.298	880	886	889	rBV	3149474	3234905	53.88%	7.757%
8	8.016	1004	1008	1011	rBV	2023253	1606290	26.75%	3.852%
9	9.098	1185	1192	1195	rBV	6275524	5766627	96.04%	13.829%
10	9.769	1302	1306	1309	rBV	2433891	1880387	31.32%	4.509%
11	10.480	1424	1427	1431	rVB	699994	543947	9.06%	1.304%
12	10.557	1435	1440	1443	rBV	3863065	3734113	62.19%	8.955%
13	10.786	1476	1479	1486	rVB	116071	92133	1.53%	0.221%
14	11.251	1554	1558	1561	rBV	2357188	1965675	32.74%	4.714%
15	11.786	1645	1649	1663	rBV	548431	545886	9.09%	1.309%
16	12.568	1779	1782	1793	rBV	89198	102207	1.70%	0.245%
17	12.839	1823	1828	1831	rBV	5906389	6004391	100.00%	14.399%
18	13.851	1987	2000	2001	rBV5	73837	210919	3.51%	0.506%
19	13.880	2001	2005	2016	rVV	1721408	1754218	29.22%	4.207%
20	13.980	2016	2022	2028	rVB	111393	156026	2.60%	0.374%
21	15.304	2241	2247	2253	rBV	1068328	1246368	20.76%	2.989%

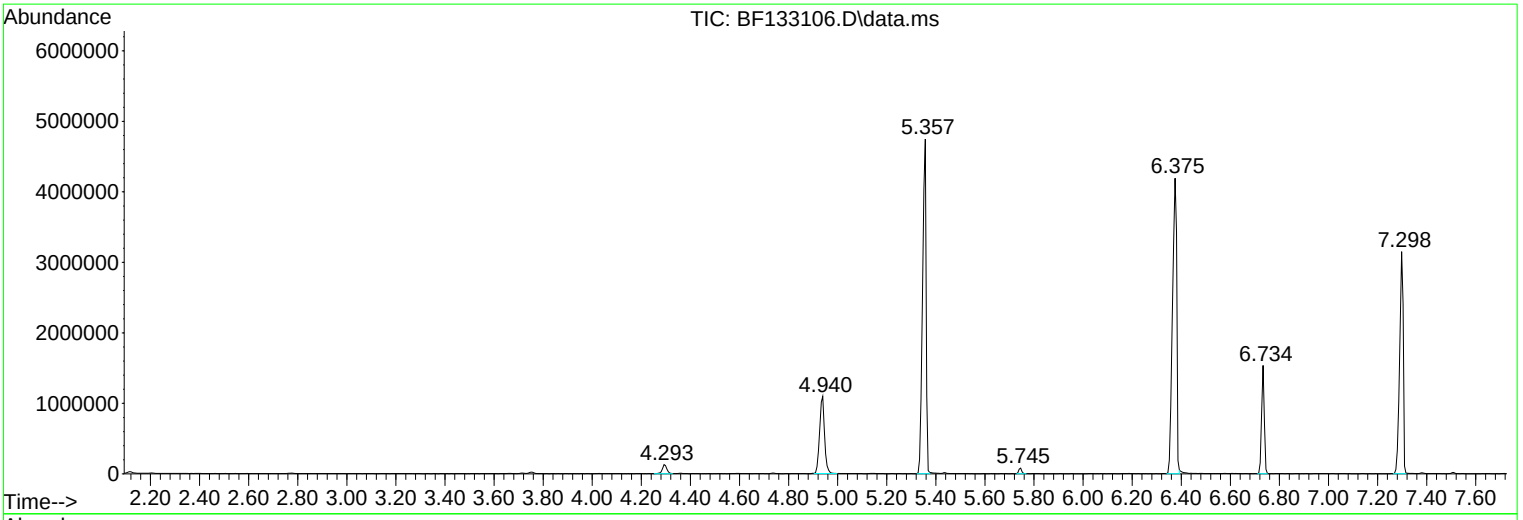
Sum of corrected areas: 41700868

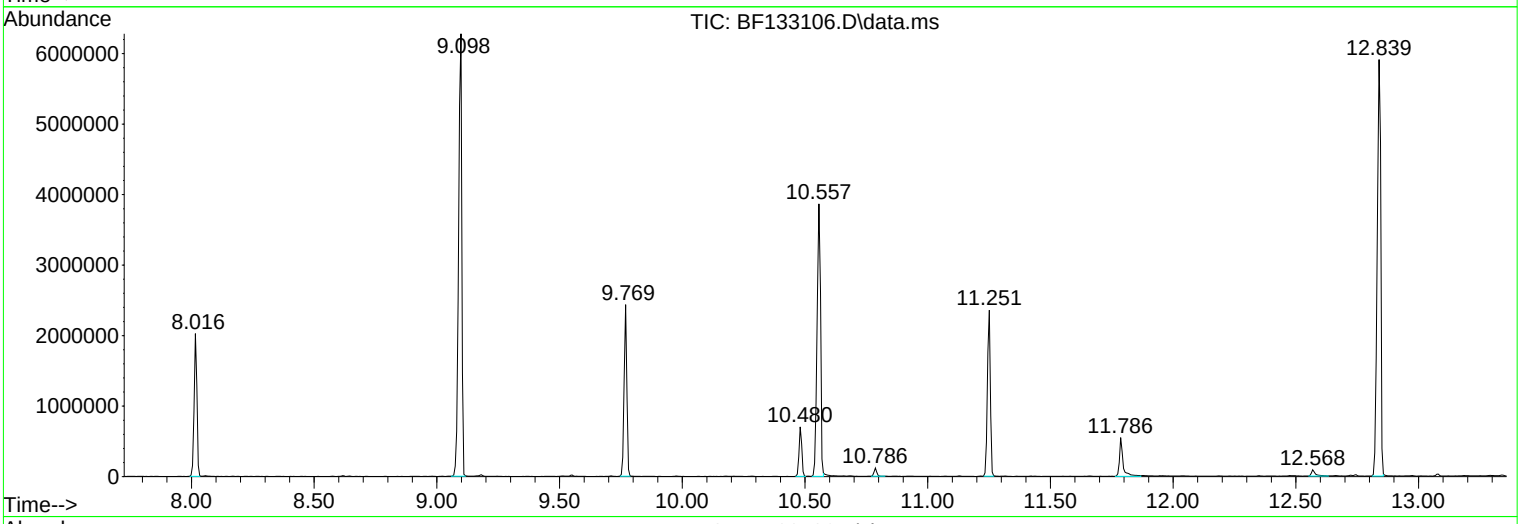
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133106.D
Acq On : 27 Apr 2023 18:25
Operator : CG\JU
Sample : 02502-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

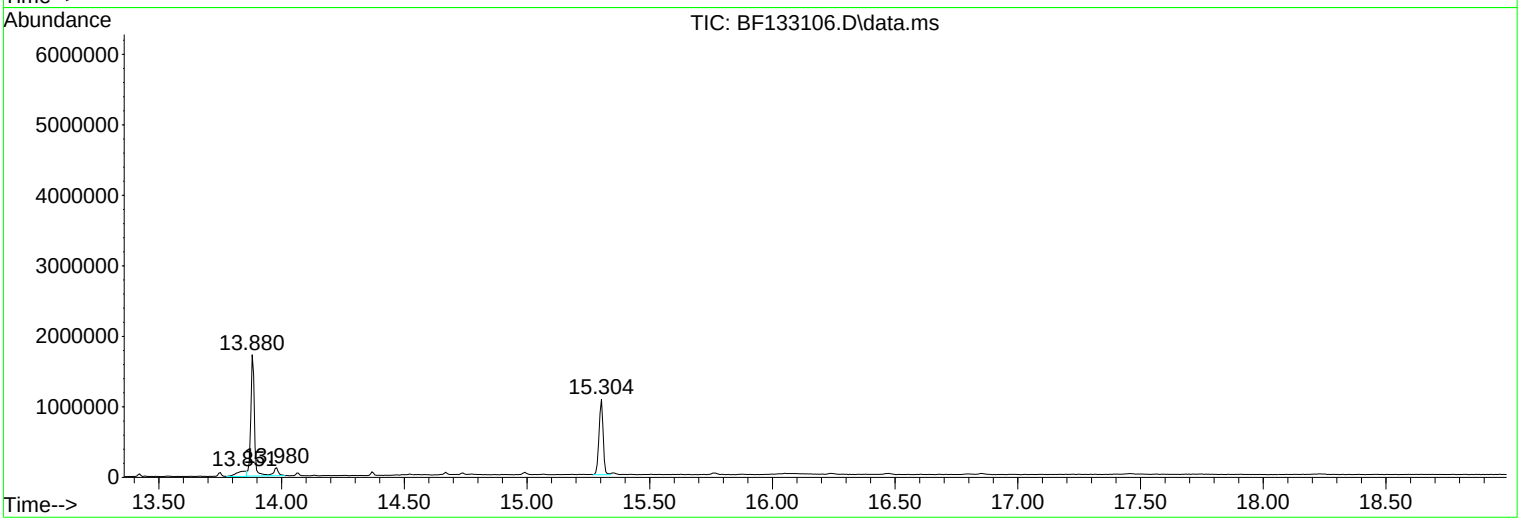
Instrument :
BNA_F
ClientSampleId :
BU-511-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133106.D
Acq On : 27 Apr 2023 18:25
Operator : CG\JU
Sample : 02502-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-511-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

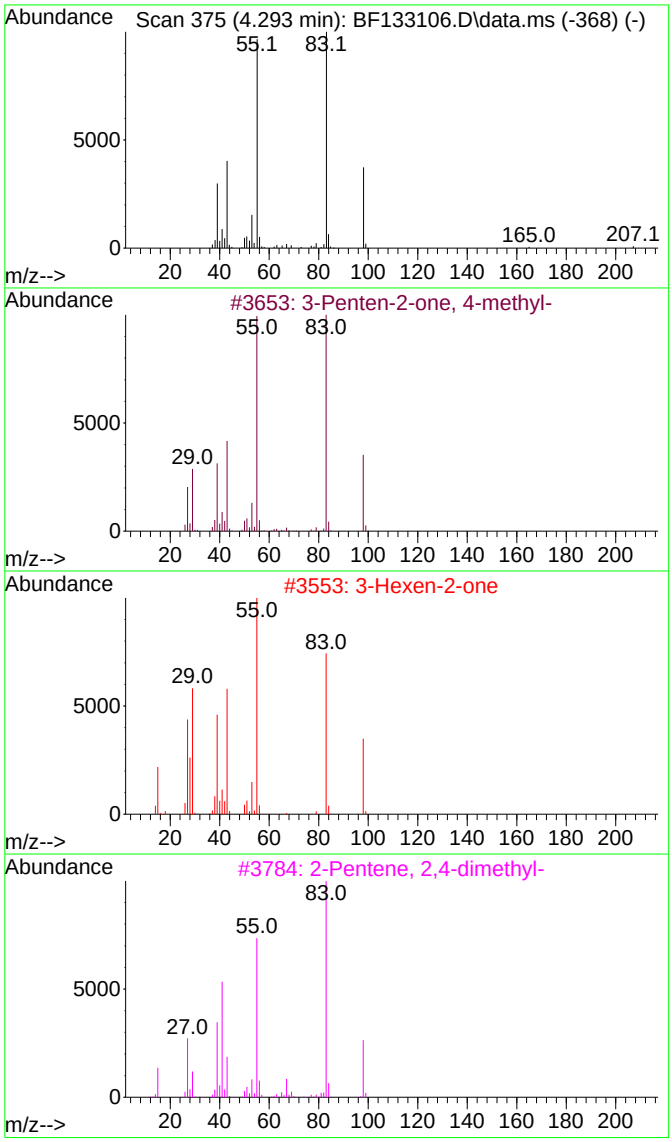
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

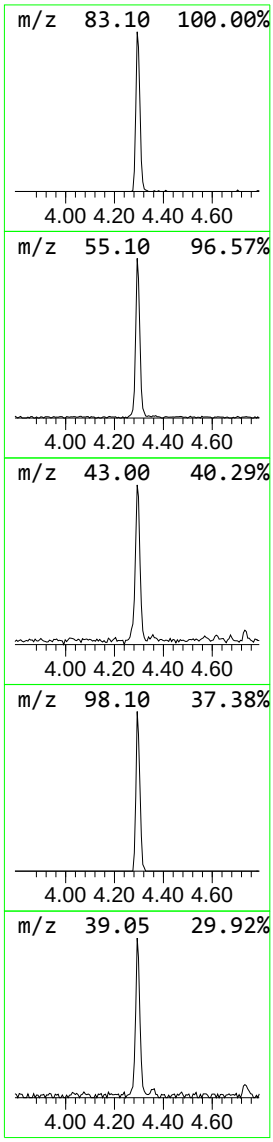
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.293	2.81 ng	164359	1,4-Dichlorobenzene-d4	6.734

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	87
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133106.D
Acq On : 27 Apr 2023 18:25
Operator : CG\JU
Sample : 02502-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-511-COMP-02

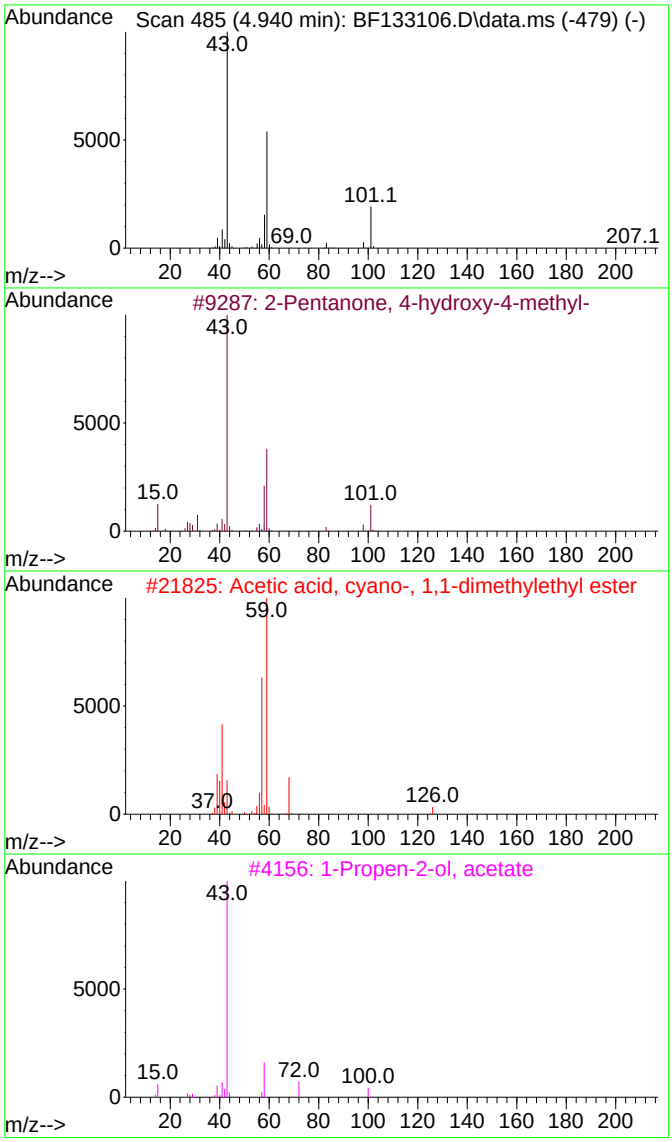
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

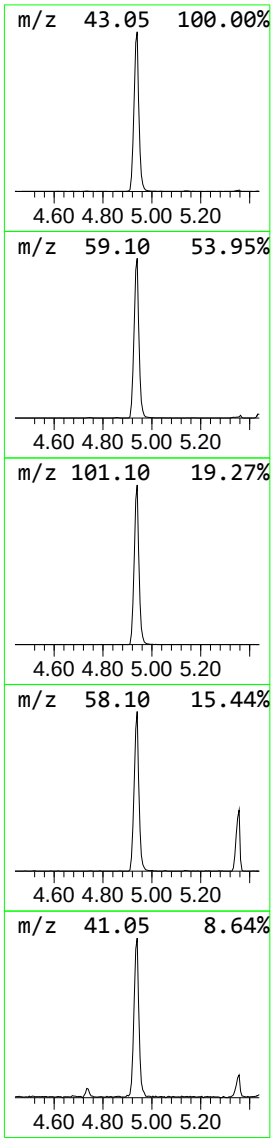
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.940	26.02 ng	1522860	1,4-Dichlorobenzene-d4	6.734

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133106.D
Acq On : 27 Apr 2023 18:25
Operator : CG\JU
Sample : 02502-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-511-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

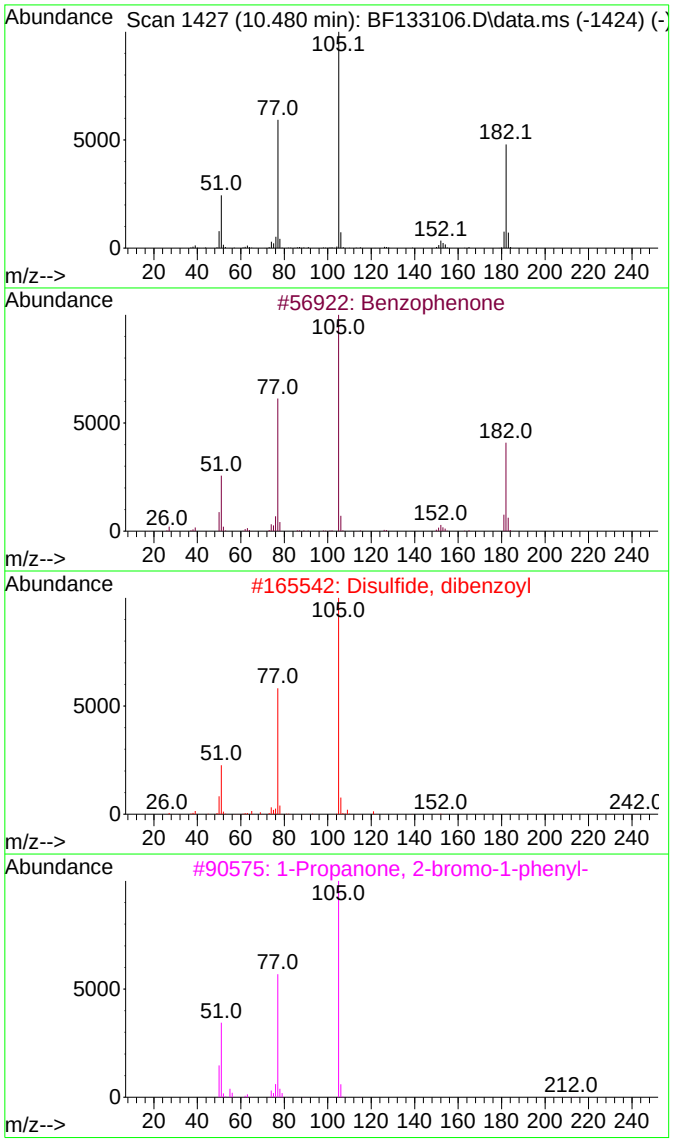
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

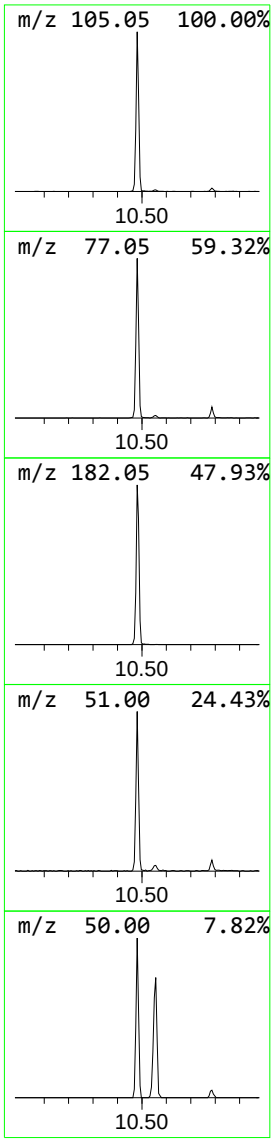
****

Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.480	5.79 ng	543947	Acenaphthene-d10	9.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
5	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133106.D
Acq On : 27 Apr 2023 18:25
Operator : CG\JU
Sample : 02502-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-511-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

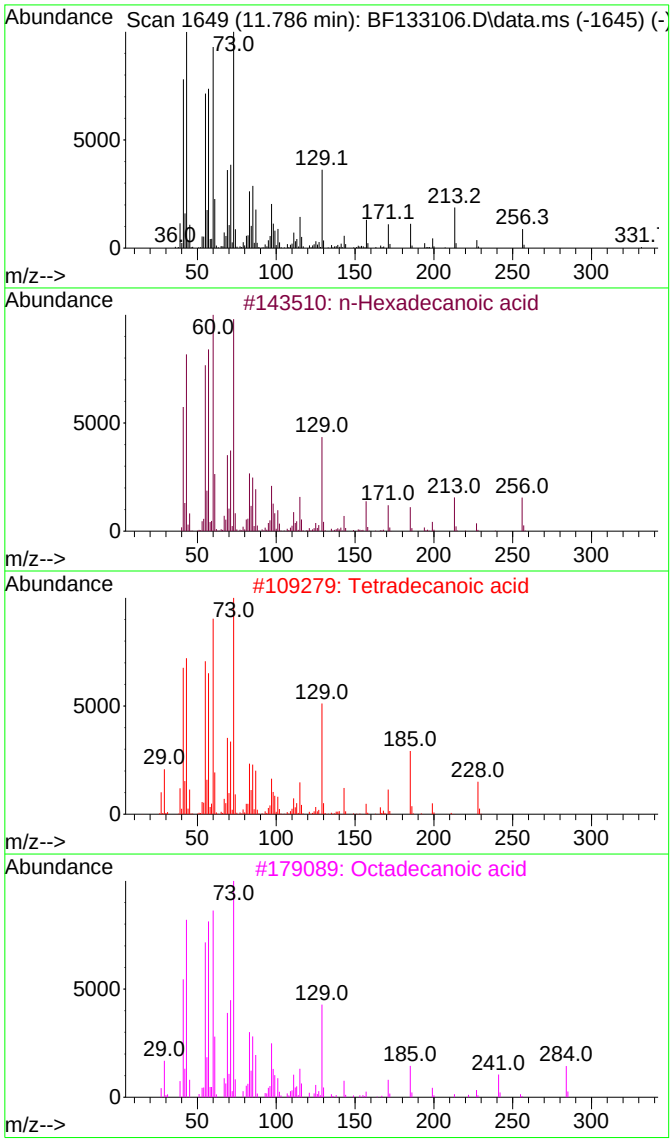
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

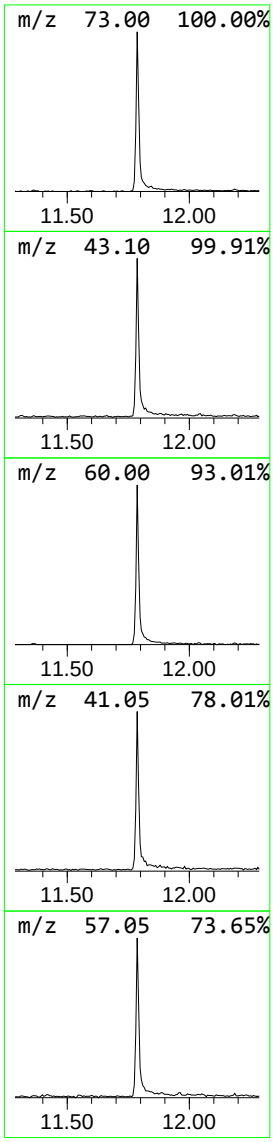
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	5.55 ng	545886	Phenanthrene-d10	11.251

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	95
3	Octadecanoic acid	284	C18H36O2	000057-11-4	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	87
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042723\
Data File : BF133106.D
Acq On : 27 Apr 2023 18:25
Operator : CG\JU
Sample : 02502-08
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BU-511-COMP-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
3-Penten-2-one,...	4.293	2.8	ng	164359	1	6.734	1170420	20.0
2-Pentanone, 4-...	4.940	26.0	ng	1522860	1	6.734	1170420	20.0
Benzophenone	10.480	5.8	ng	543947	3	9.769	1880390	20.0
n-Hexadecanoic ...	11.786	5.5	ng	545886	4	11.251	1965680	20.0