LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060523\
Data File : BF133568.D
Acq On : 05 Jun 2023 16:28
Operator : CG\JU
Sample : 02998-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-2-053123

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-BF052523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133568.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	6	13	19	rBV	31530	45044	1.84%	0.246%
2	5.034	497	501	508	rBV	85476	99342	4.06%	0.542%
3	5.440	565	570	573	rBV	2275124	2227952	91.00%	12.163%
4	6.457	737	743	746	rBV	2161541	2249538	91.88%	12.281%
5	6.834	803	807	810	rBV	1102552	899988	36.76%	4.913%
6	7.392	898	902	905	rBV	1682369	1379971	56.36%	7.534%
7	8.116	1021	1025	1028	rBV	1434752	1110798	45.37%	6.064%
8	9.192	1204	1208	1211	rBV	3125106	2448433	100.00%	13.366%
9	9.869	1320	1323	1327	rBV	1328963	1062534	43.40%	5.801%
10	10.586	1441	1445	1447	rBV	138792	123080	5.03%	0.672%
11	10.657	1453	1457	1460	rBV	1584229	1317336	53.80%	7.192%
12	10.780	1472	1478	1479	rBV2	28563	45299	1.85%	0.247%
13	11.357	1572	1576	1579	rBV	1302364	1043065	42.60%	5.694%
14	11.380	1579	1580	1583	rVB	79902	43657	1.78%	0.238%
15	11.886	1663	1666	1671	rBV	328486	309482	12.64%	1.690%
16	12.568	1779	1782	1785	rBV	176003	164398	6.71%	0.897%
17	12.674	1797	1800	1804	rBV2	104464	110784	4.52%	0.605%
18	12.798	1818	1821	1824	rBV	148303	121057	4.94%	0.661%
19	12.951	1842	1847	1850	rBV	2188929	2084296	85.13%	11.379%
20	13.180	1884	1886	1890	rBV4	50328	67593	2.76%	0.369%
21	13.998	2021	2025	2028	rBV2	740795	814796	33.28%	4.448%
22	15.462	2270	2274	2277	rBV	454084	549271	22.43%	2.999%

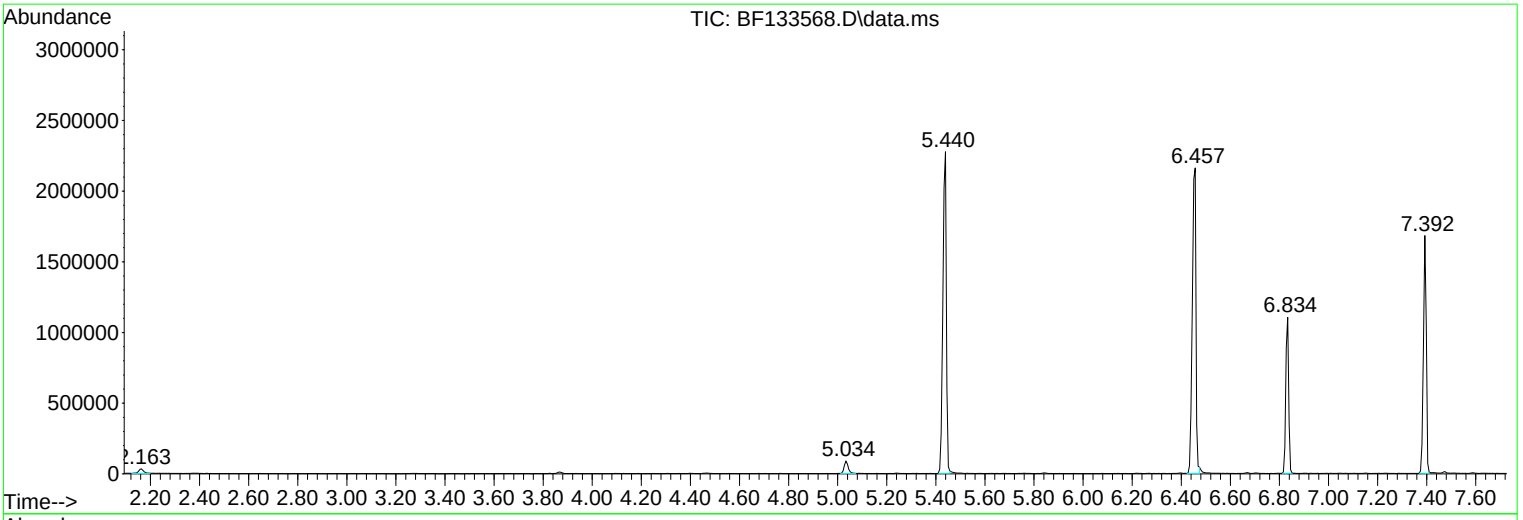
Sum of corrected areas: 18317714

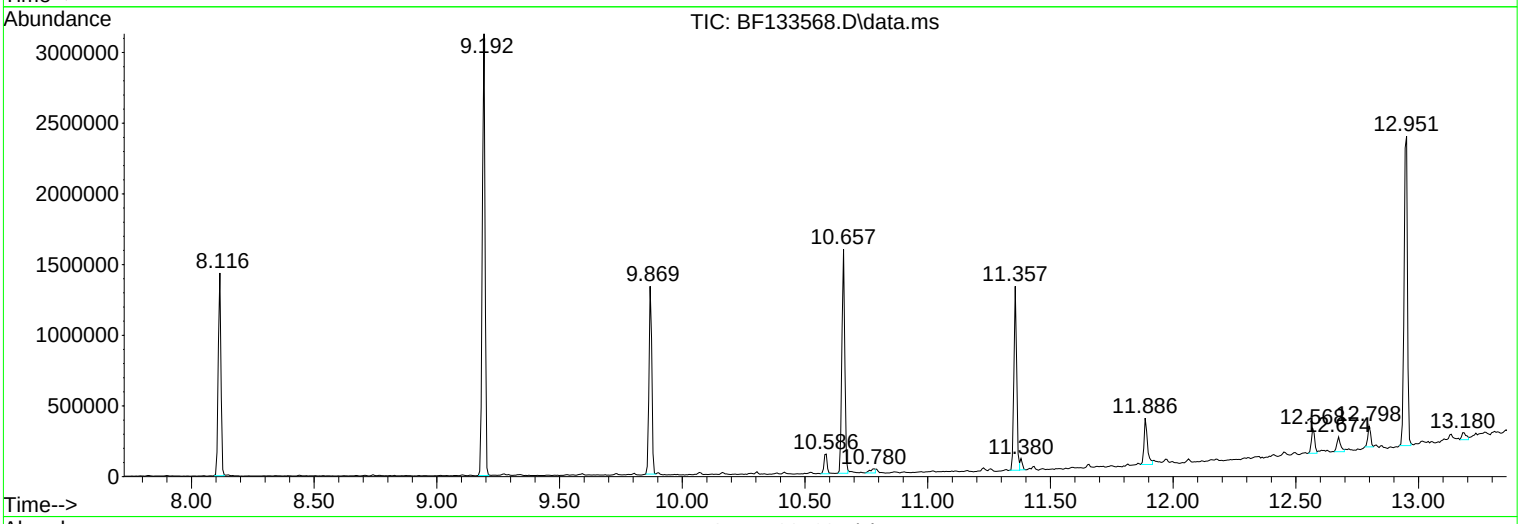
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060523\
Data File : BF133568.D
Acq On : 05 Jun 2023 16:28
Operator : CG\JU
Sample : 02998-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

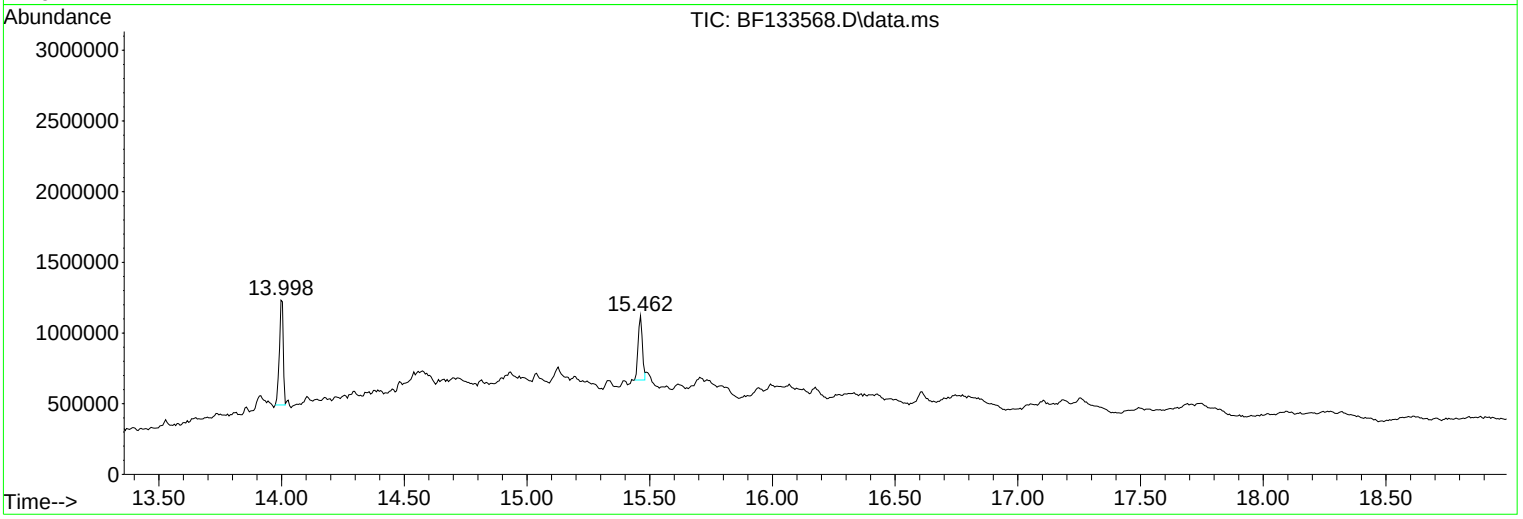
Instrument :
BNA_F
ClientSampleId :
PAT-2-053123

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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\BF060523\
Data File : BF133568.D
Acq On : 05 Jun 2023 16:28
Operator : CG\JU
Sample : 02998-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-2-053123

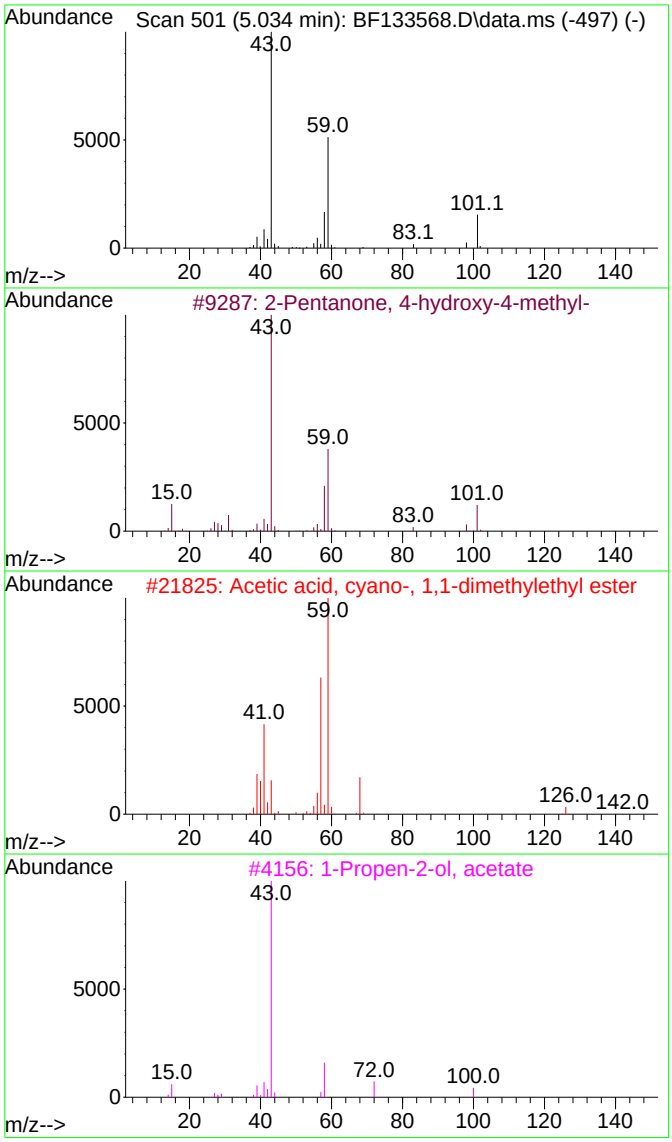
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

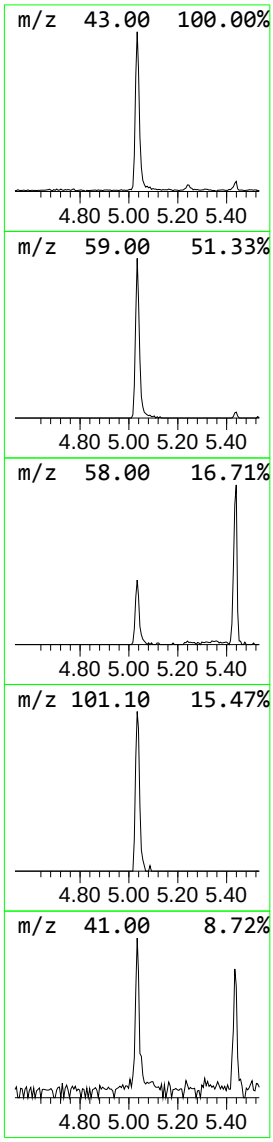
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.034	2.21 ng	99342	1,4-Dichlorobenzene-d4	6.834

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060523\
Data File : BF133568.D
Acq On : 05 Jun 2023 16:28
Operator : CG\JU
Sample : 02998-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-2-053123

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

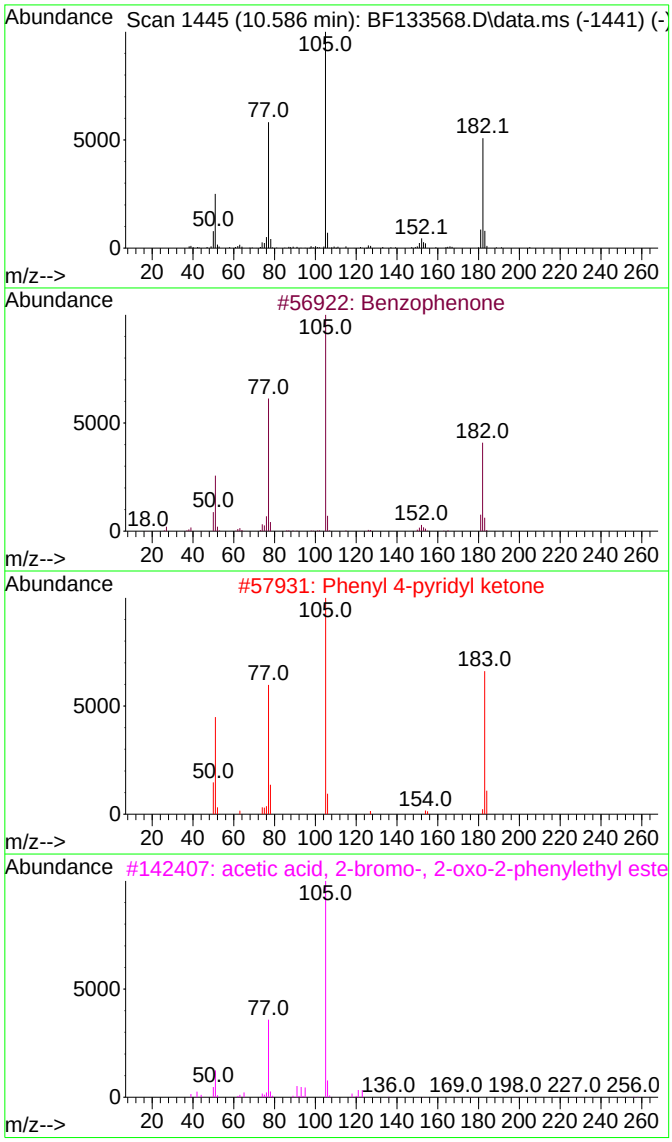
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

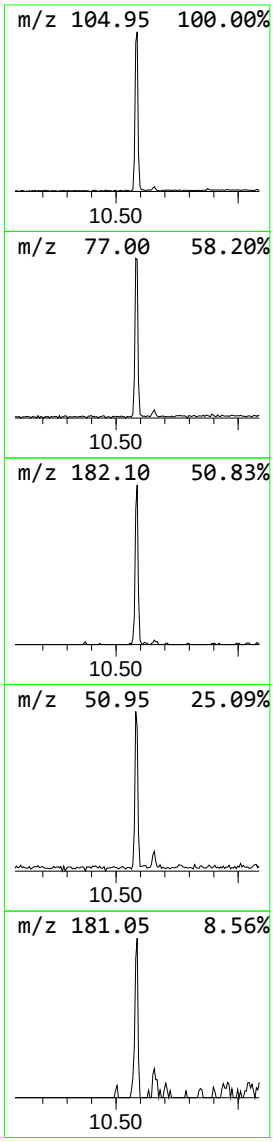
****

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.586	2.32 ng	123080	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3	acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47
4	1,2,4-Triazine-3,5(2H,4H)-dione,...	249	C10H7N3O3S	024168-34-1	47
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060523\
Data File : BF133568.D
Acq On : 05 Jun 2023 16:28
Operator : CG\JU
Sample : 02998-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-2-053123

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

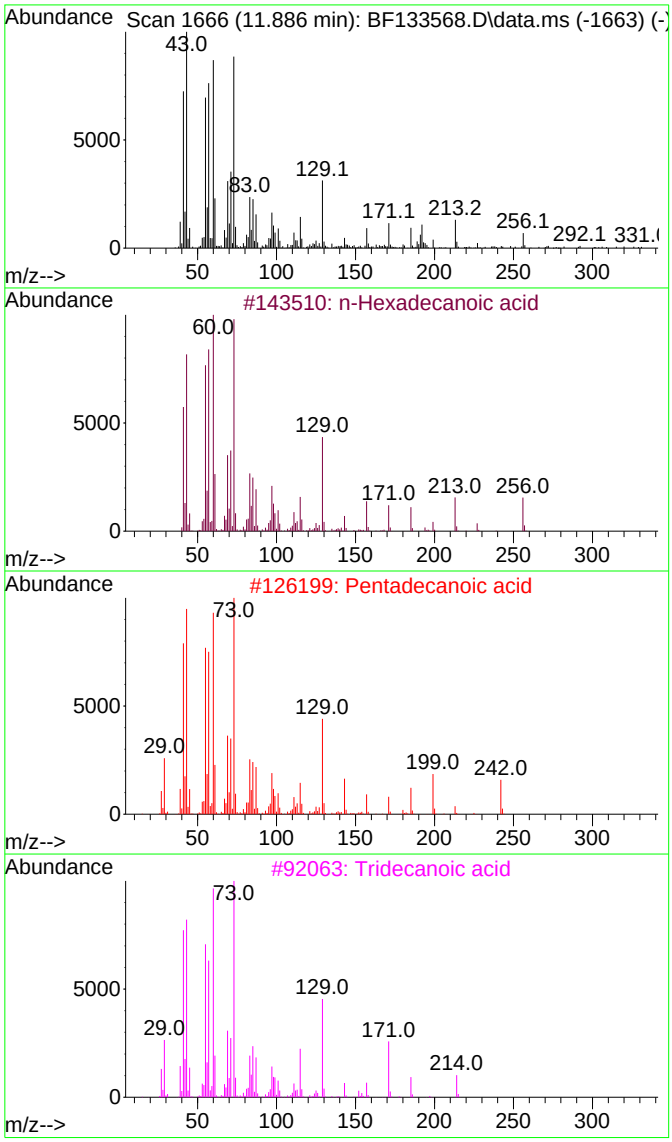
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

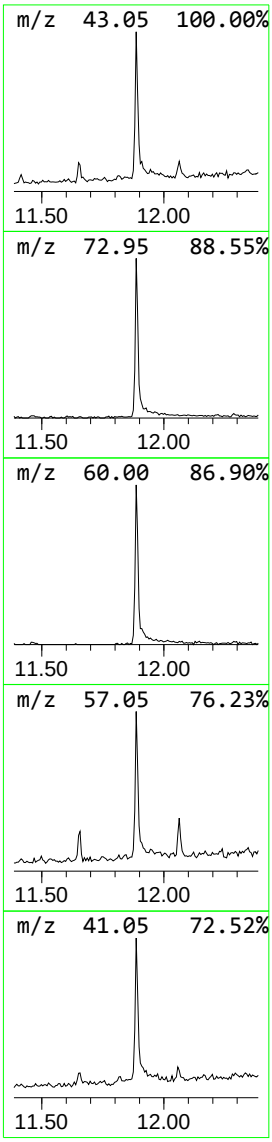
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	5.93 ng	309482	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	94
4	Octadecanoic acid	284	C18H36O2	000057-11-4	81
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060523\
Data File : BF133568.D
Acq On : 05 Jun 2023 16:28
Operator : CG\JU
Sample : 02998-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-2-053123

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

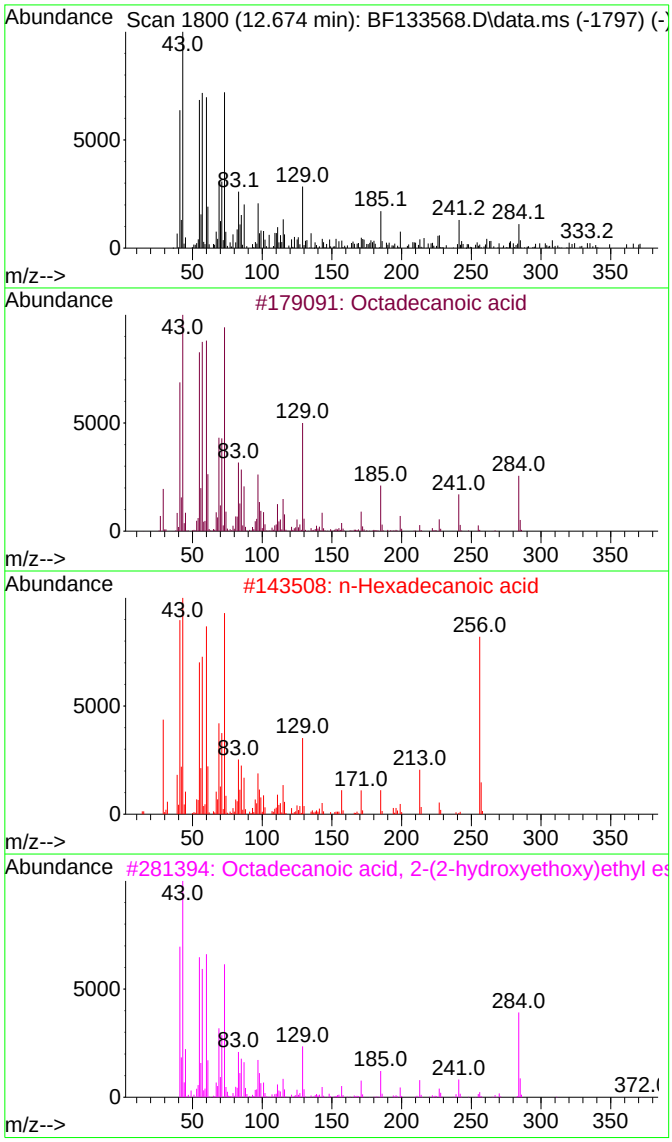
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

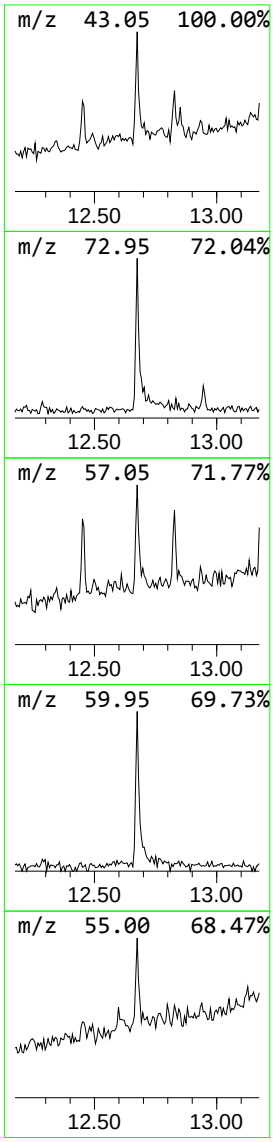
****

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.674	2.12 ng	110784	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
4	Eicosanoic acid	312	C20H40O2	000506-30-9	60
5	Pentadecanoic acid, 15-bromo-	320	C15H29BrO2	056523-59-2	60





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060523\
Data File : BF133568.D
Acq On : 05 Jun 2023 16:28
Operator : CG\JU
Sample : 02998-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAT-2-053123

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.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-...	5.034	2.2	ng	99342	1	6.834	899988	20.0
Benzophenone	10.586	2.3	ng	123080	3	9.869	1062530	20.0
n-Hexadecanoic ...	11.886	5.9	ng	309482	4	11.357	1043070	20.0
Octadecanoic acid	12.674	2.1	ng	110784	4	11.357	1043070	20.0