LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019827.D
Acq On : 22 Feb 2024 16:40
Operator : MA/JU
Sample : P1521-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : CG-MW-23

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_P\Methods\8270E-BP013124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019827.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	320	328	336	rBV	72746	108472	2.30%	0.562%
2	5.469	398	405	416	rBV	451304	690458	14.66%	3.579%
3	7.069	669	677	691	rBV	235861	405261	8.60%	2.101%
4	7.893	808	817	824	rBV	232219	383897	8.15%	1.990%
5	9.063	1009	1016	1027	rBV	672801	1197514	25.42%	6.207%
6	10.693	1284	1293	1302	rBV	286046	503748	10.69%	2.611%
7	12.345	1564	1574	1581	rBV2	26277	57778	1.23%	0.299%
8	13.157	1705	1712	1725	rBV	1886752	2920514	61.99%	15.138%
9	14.363	1909	1917	1926	rVB2	22042	51761	1.10%	0.268%
10	14.534	1939	1946	1953	rBV	444965	718418	15.25%	3.724%
11	14.598	1953	1957	1968	rVB2	38922	87081	1.85%	0.451%
12	16.028	2194	2200	2211	rBV	2284363	3397231	72.11%	17.610%
13	17.057	2371	2375	2380	rBV	42443	57698	1.22%	0.299%
14	17.292	2409	2415	2420	rBV	627629	881543	18.71%	4.569%
15	18.186	2562	2567	2575	rBV	353023	500218	10.62%	2.593%
16	19.422	2774	2777	2781	rBV2	95961	121259	2.57%	0.629%
17	19.857	2846	2851	2857	rBV	3825160	4711179	100.00%	24.420%
18	21.104	3060	3063	3068	rVB	290348	333523	7.08%	1.729%
19	21.386	3106	3111	3117	rBV	761655	1039818	22.07%	5.390%
20	23.804	3517	3522	3533	rVB	513898	1124614	23.87%	5.829%

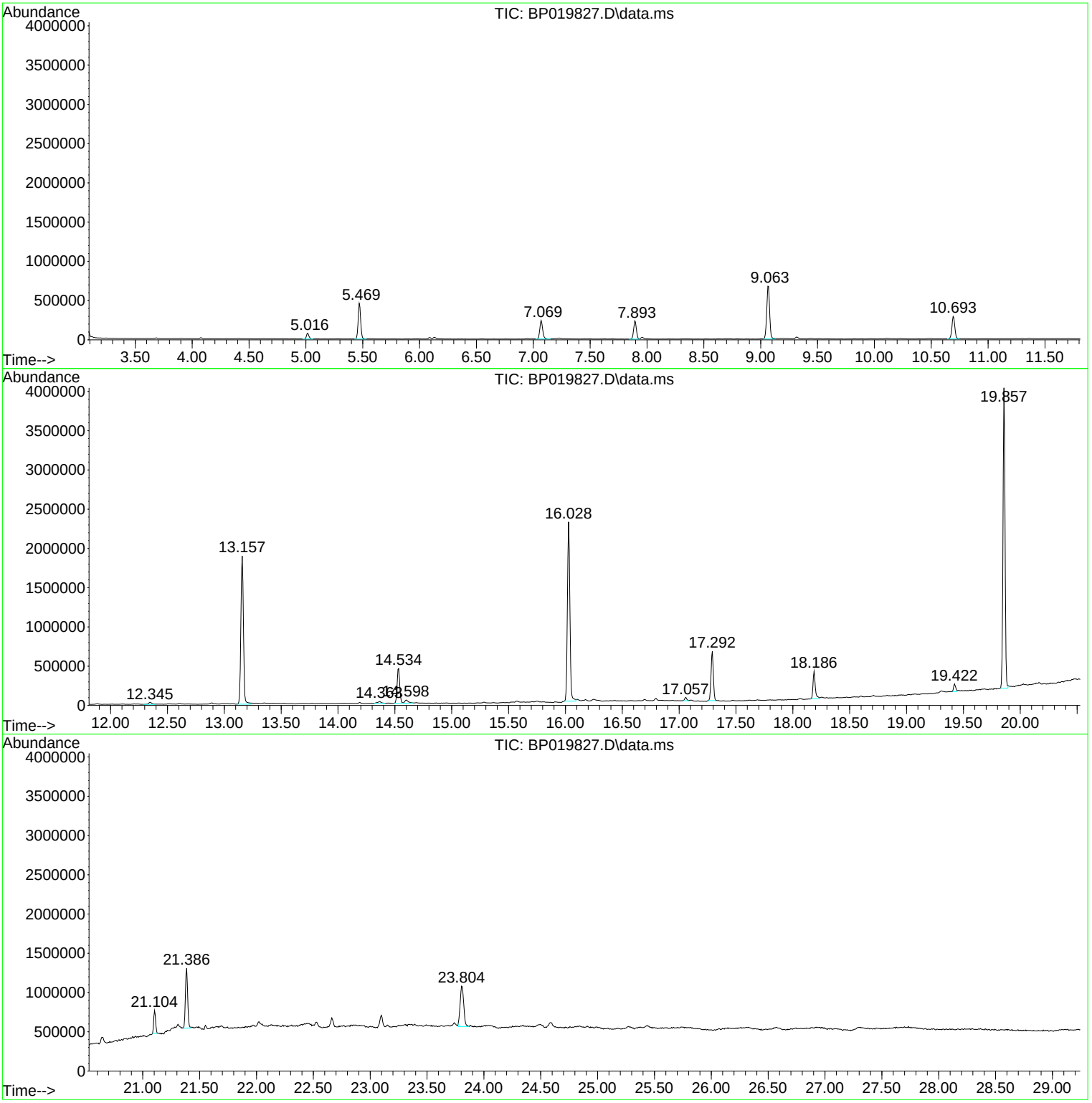
Sum of corrected areas: 19291985

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019827.D
Acq On : 22 Feb 2024 16:40
Operator : MA/JU
Sample : P1521-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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_P\Data\BP022224\
Data File : BP019827.D
Acq On : 22 Feb 2024 16:40
Operator : MA/JU
Sample : P1521-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-23

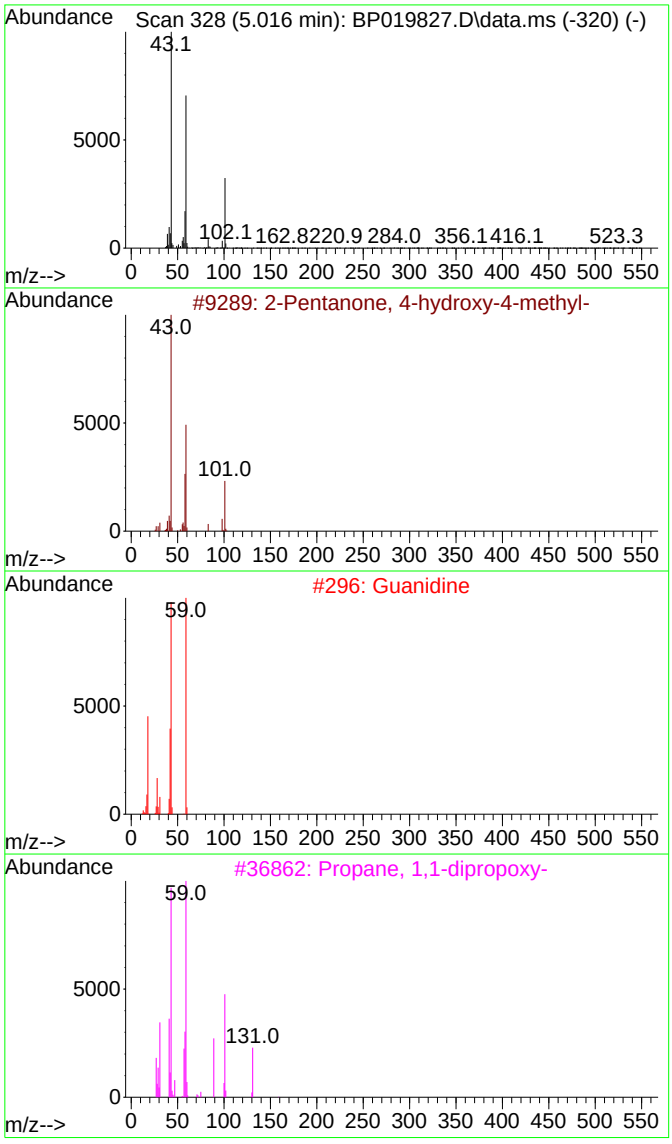
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

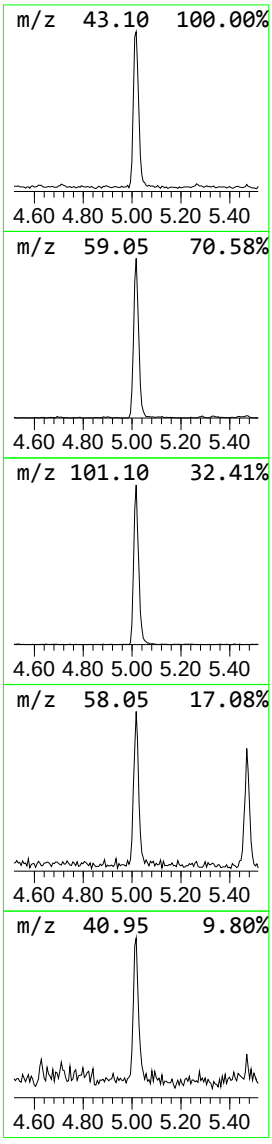
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	5.65 ng	108472	1,4-Dichlorobenzene-d4	7.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Guanidine	59	CH5N3	000113-00-8	43
3	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	38
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	36
5	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019827.D
Acq On : 22 Feb 2024 16:40
Operator : MA/JU
Sample : P1521-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

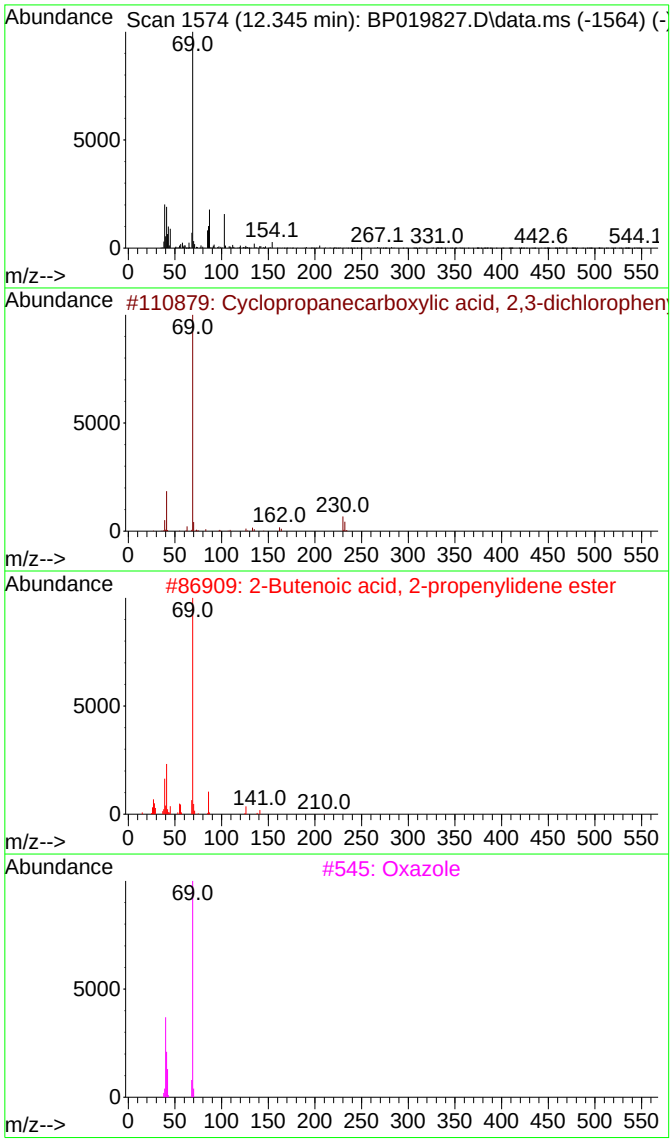
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

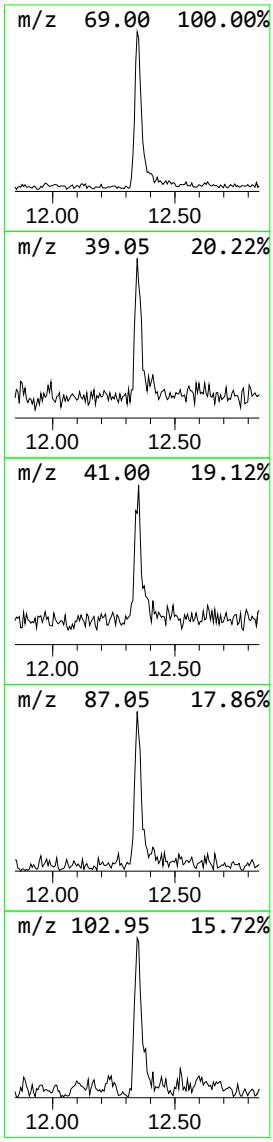
****

Peak Number 2 Cyclopropanecarboxylic acid... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.345	2.29 ng	57778	Naphthalene-d8	10.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropanecarboxylic acid, 2,3...	230	C10H8Cl2O2	959085-02-0	50
2	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	36
3	Oxazole	69	C3H3NO	000288-42-6	9
4	Vinyl crotonate	112	C6H8O2	014861-06-4	9
5	5,6-Decanediol	174	C10H22O2	054884-84-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019827.D
Acq On : 22 Feb 2024 16:40
Operator : MA/JU
Sample : P1521-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

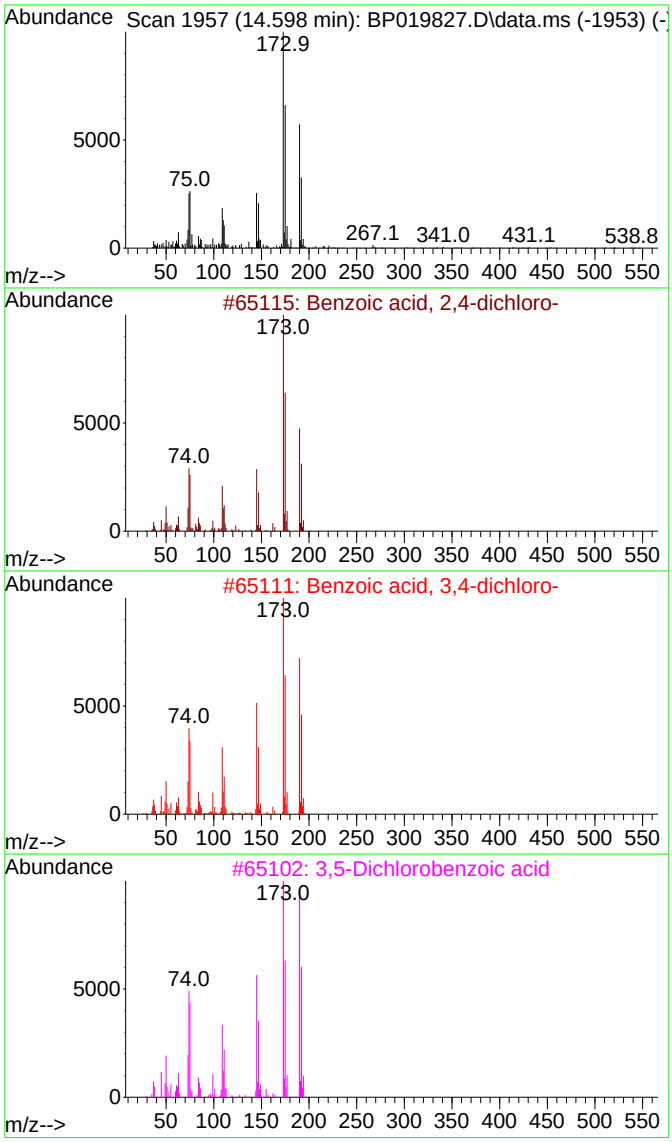
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

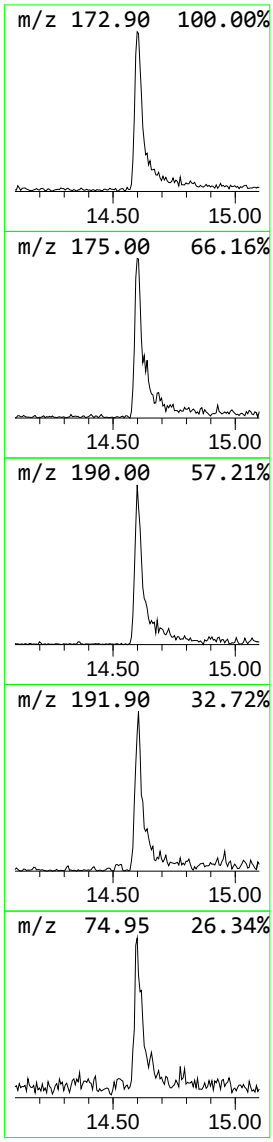
****

Peak Number 3 Benzoic acid, 2,4-dichloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.598	2.42 ng	87081	Acenaphthene-d10	14.534

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2,4-dichloro-	190	C7H4Cl2O2	000050-84-0	95
2	Benzoic acid, 3,4-dichloro-	190	C7H4Cl2O2	000051-44-5	95
3	3,5-Dichlorobenzoic acid	190	C7H4Cl2O2	000051-36-5	95
4	Benzoic acid, 2,5-dichloro-	190	C7H4Cl2O2	000050-79-3	94
5	Benzoic acid, 2,6-dichloro-	190	C7H4Cl2O2	000050-30-6	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019827.D
Acq On : 22 Feb 2024 16:40
Operator : MA/JU
Sample : P1521-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

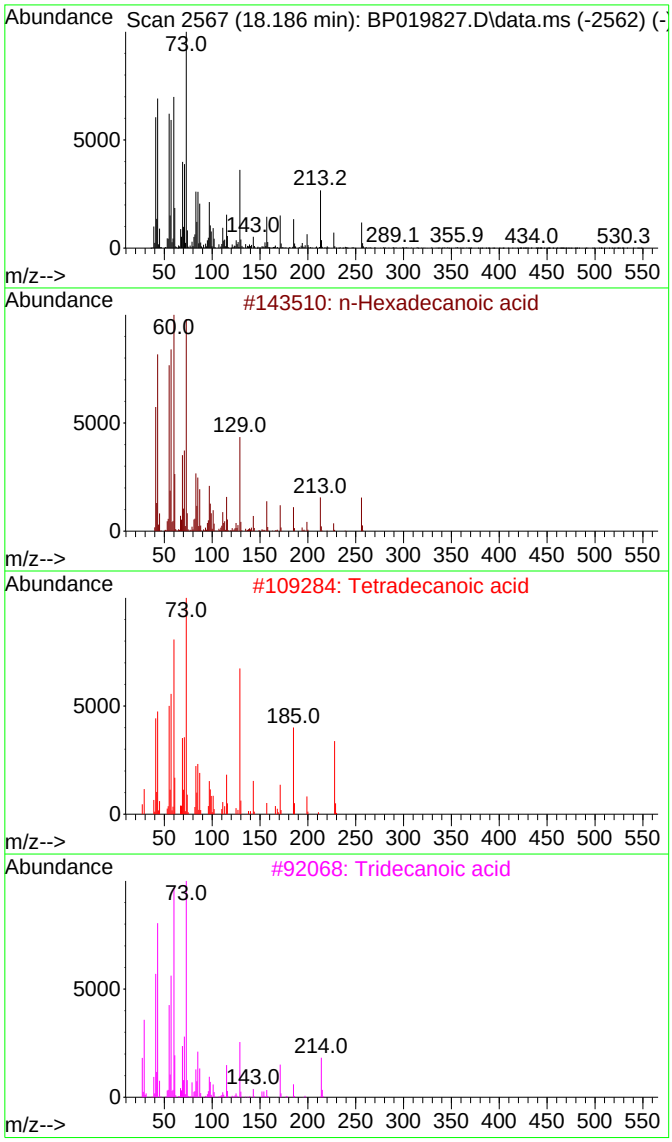
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

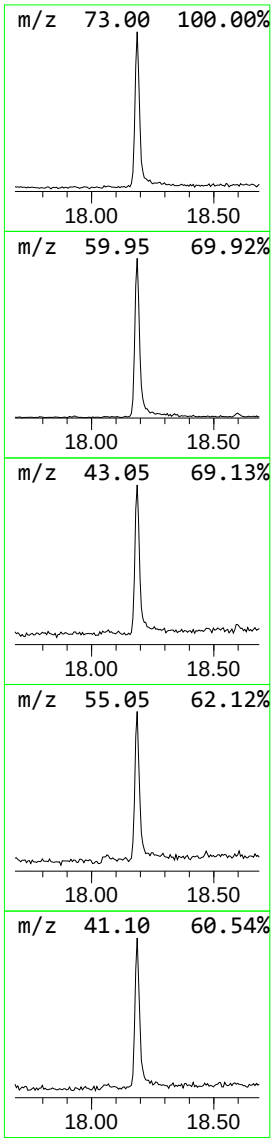
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.186	11.35 ng	500218	Phenanthrene-d10	17.292

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	86
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Octadecanoic acid	284	C18H36O2	000057-11-4	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019827.D
Acq On : 22 Feb 2024 16:40
Operator : MA/JU
Sample : P1521-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

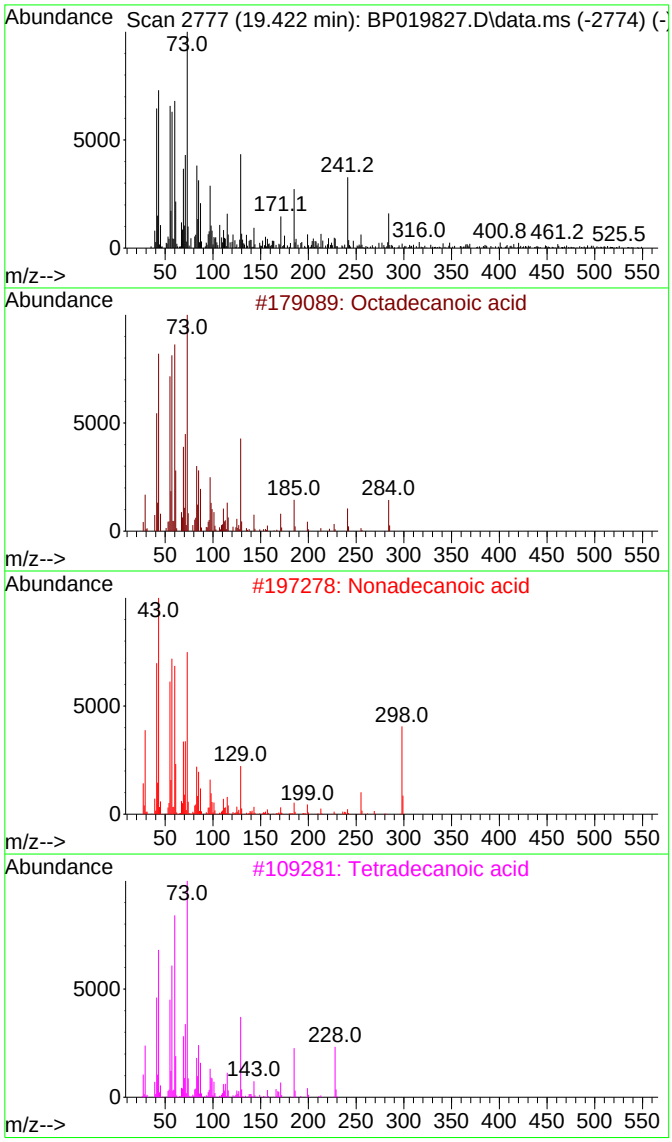
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

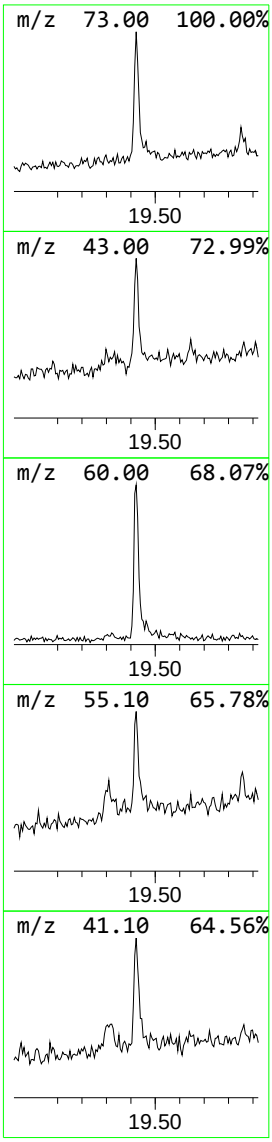
****

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.422	2.33 ng	121259	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Nonadecanoic acid	298	C19H38O2	000646-30-0	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
5	Tetracosanoic acid	368	C24H48O2	000557-59-5	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019827.D
Acq On : 22 Feb 2024 16:40
Operator : MA/JU
Sample : P1521-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-23

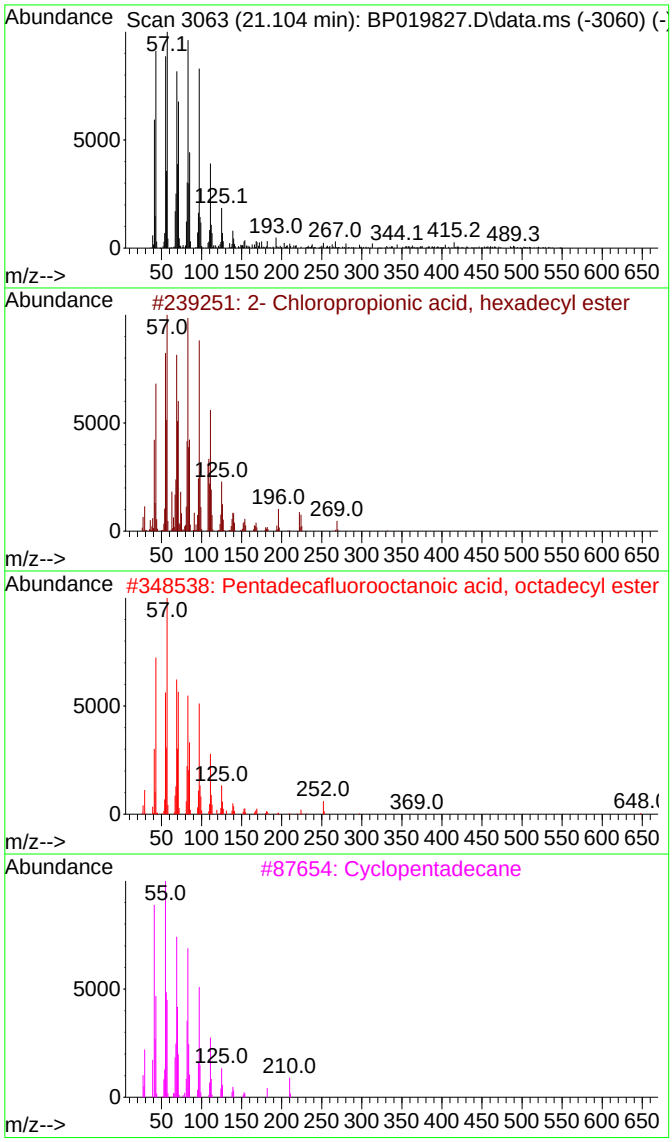
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

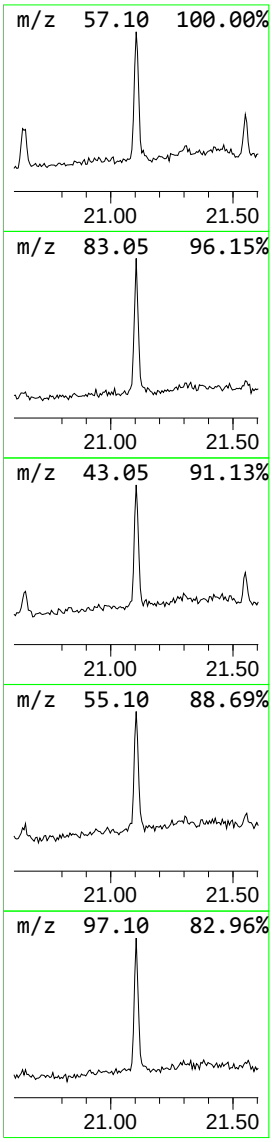
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2- Chloropropionic acid, he... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.104	6.42 ng	333523	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	94
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
3	Cyclopentadecane	210	C15H30	000295-48-7	92
4	1-Tetracosene	336	C24H48	010192-32-2	91
5	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019827.D
Acq On : 22 Feb 2024 16:40
Operator : MA/JU
Sample : P1521-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-23

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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-...	5.016	5.7	ng	108472	1	7.893	383897	20.0
Cyclopropanecar...	12.345	2.3	ng	57778	2	10.693	503748	20.0
Benzoic acid, 2...	14.598	2.4	ng	87081	3	14.534	718418	20.0
n-Hexadecanoic ...	18.186	11.4	ng	500218	4	17.292	881543	20.0
Octadecanoic acid	19.422	2.3	ng	121259	5	21.386	1039820	20.0
2- Chloropropio...	21.104	6.4	ng	333523	5	21.386	1039820	20.0