LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035297.D
Acq On : 27 May 2022 20:03
Operator : CG/JU
Sample : N2930-21
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P006-SS002-2430-01

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_M\Methods\8270-BM052722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035297.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	% max.	% of total
1	4.993	319	324	331	rVB2	43392	64208	1.33%	0.236%
2	5.457	396	403	422	rBV	1491329	2183232	45.29%	8.008%
3	7.051	665	674	687	rBV	1338743	2200756	45.65%	8.073%
4	7.875	807	814	823	rBV	434764	688148	14.27%	2.524%
5	9.034	1004	1011	1025	rBV	845561	1422884	29.51%	5.219%
6	10.675	1277	1290	1303	rBV	519258	886573	18.39%	3.252%
7	13.139	1701	1709	1725	rBV	2139742	3332737	69.13%	12.225%
8	14.510	1934	1942	1961	rVB	741813	1141411	23.68%	4.187%
9	15.998	2189	2195	2203	rBV	1645805	2332841	48.39%	8.557%
10	17.257	2400	2409	2415	rBV	939202	1356808	28.14%	4.977%
11	17.880	2509	2515	2521	rBV	93967	135452	2.81%	0.497%
12	18.157	2558	2562	2571	rBV	283158	441420	9.16%	1.619%
13	19.315	2756	2759	2766	rVB	42732	63796	1.32%	0.234%
14	19.433	2775	2779	2790	rBV	241642	393733	8.17%	1.444%
15	19.674	2816	2820	2822	rBV2	36858	51692	1.07%	0.190%
16	19.880	2849	2855	2864	rBV	3934686	4820991	100.00%	17.684%
17	20.168	2900	2904	2907	rBV4	51351	69598	1.44%	0.255%
18	20.445	2947	2951	2955	rVB3	76168	91836	1.90%	0.337%
19	20.574	2970	2973	2976	rBV	87234	93857	1.95%	0.344%
20	20.909	3027	3030	3035	rVB4	68555	81089	1.68%	0.297%
21	21.133	3064	3068	3080	rBV2	527636	1096656	22.75%	4.023%
22	21.350	3102	3105	3109	rBV	130729	146685	3.04%	0.538%
23	21.433	3114	3119	3123	rBV	1322766	1741762	36.13%	6.389%
24	21.609	3145	3149	3154	rVB2	205443	314451	6.52%	1.153%
25	21.662	3155	3158	3162	rVB	234169	264342	5.48%	0.970%
26	21.968	3207	3210	3216	rVB4	139970	174961	3.63%	0.642%
27	23.797	3516	3521	3530	rVB2	828125	1670342	34.65%	6.127%

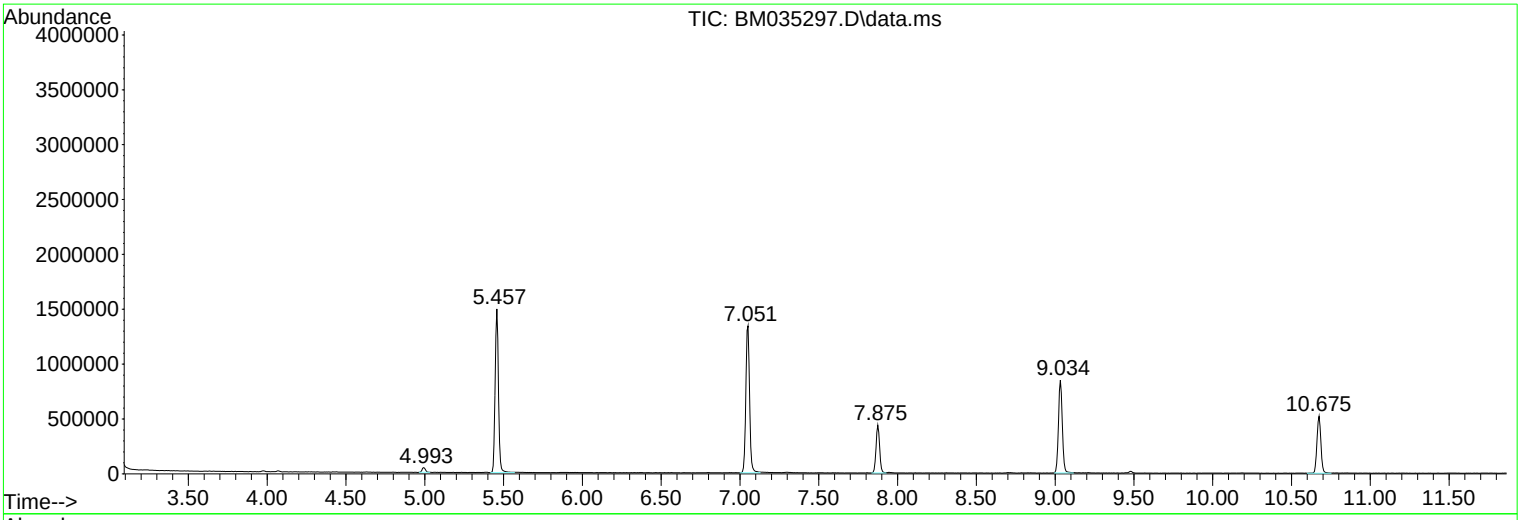
Sum of corrected areas: 27262261

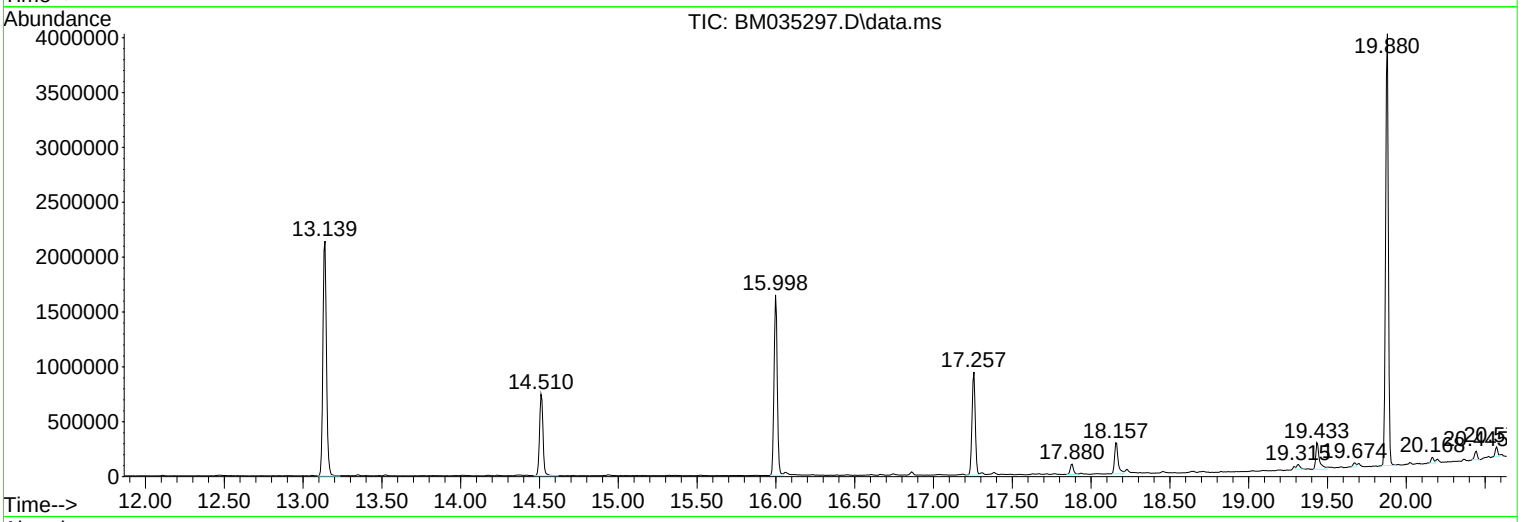
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035297.D
Acq On : 27 May 2022 20:03
Operator : CG/JU
Sample : N2930-21
Misc :
ALS Vial : 16 Sample Multiplier: 1

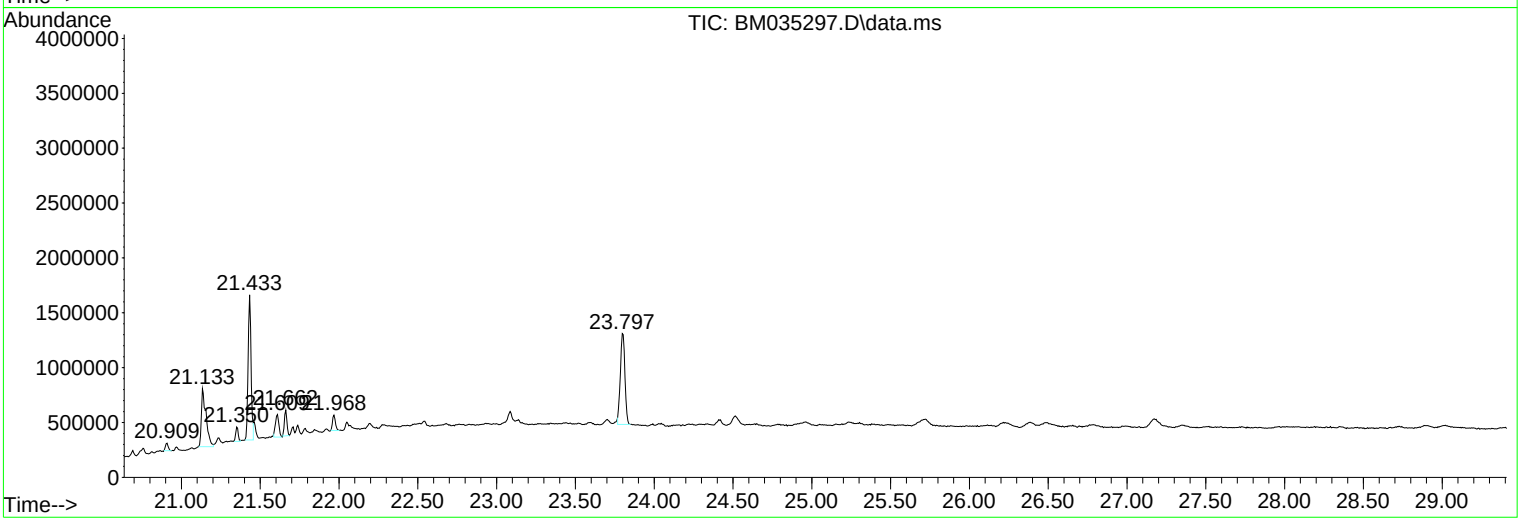
Instrument :
BNA_M
ClientSampleId :
P006-SS002-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.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_M\Data\BM052722\
Data File : BM035297.D
Acq On : 27 May 2022 20:03
Operator : CG/JU
Sample : N2930-21
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P006-SS002-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

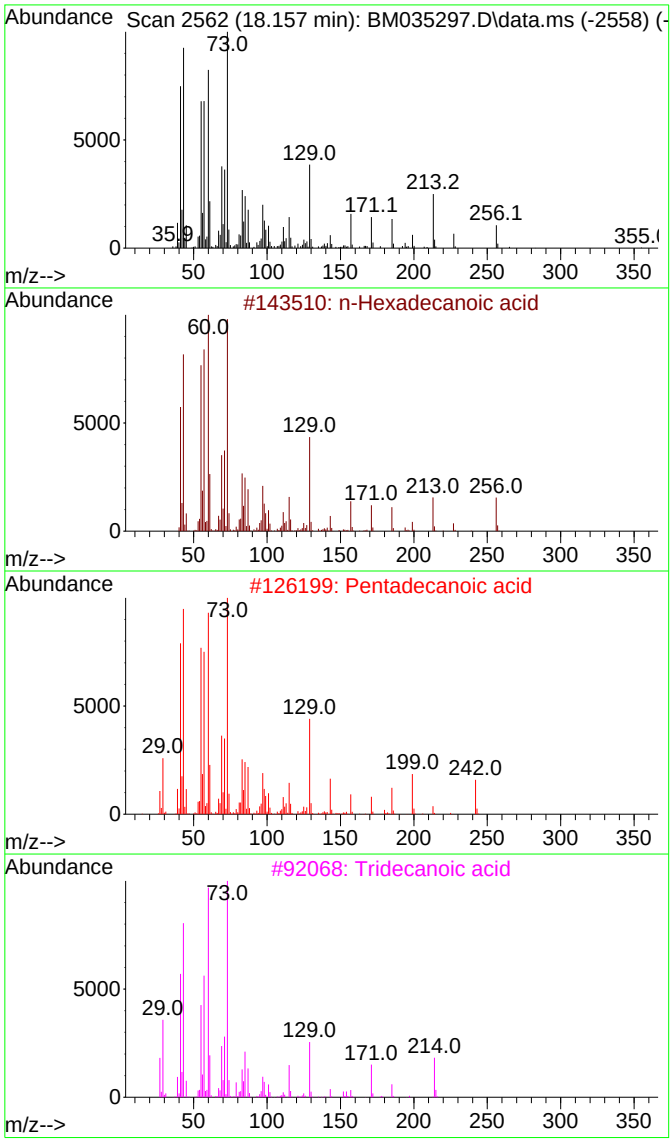
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

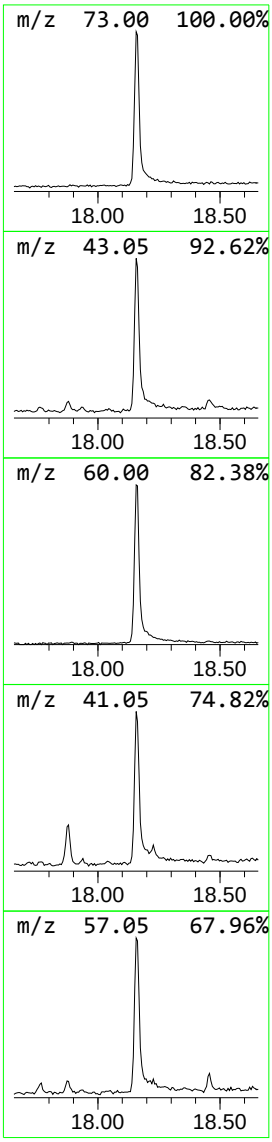
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.157	6.51 ng	441420	Phenanthrene-d10	17.257

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	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035297.D
Acq On : 27 May 2022 20:03
Operator : CG/JU
Sample : N2930-21
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P006-SS002-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

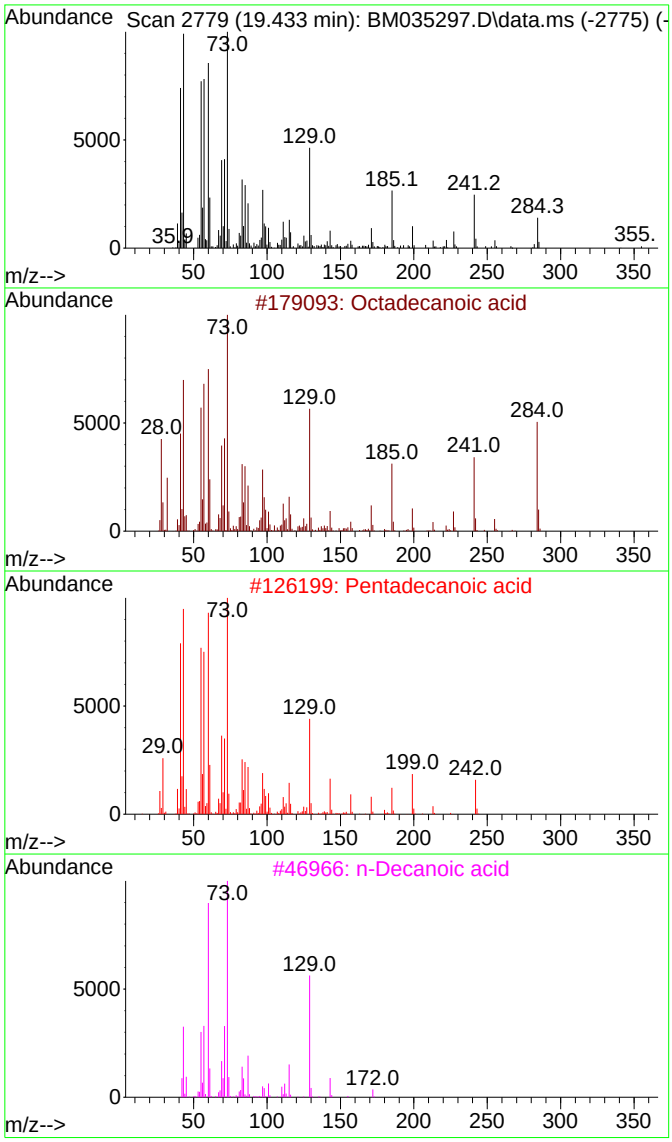
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

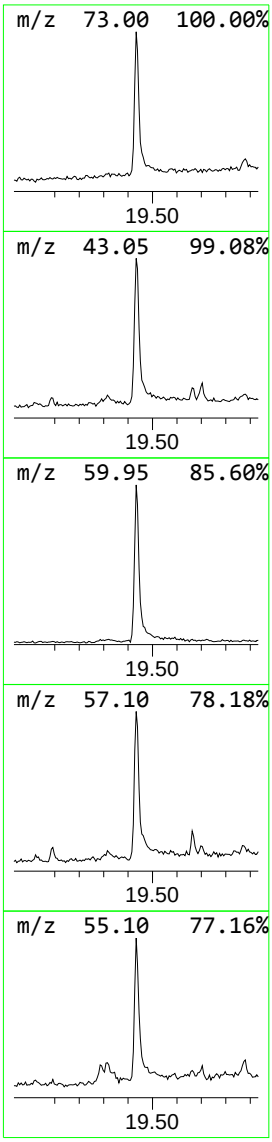
****

Peak Number 2 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.433	4.52 ng	393733	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Decanoic acid	172	C10H20O2	000334-48-5	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035297.D
Acq On : 27 May 2022 20:03
Operator : CG/JU
Sample : N2930-21
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P006-SS002-2430-01

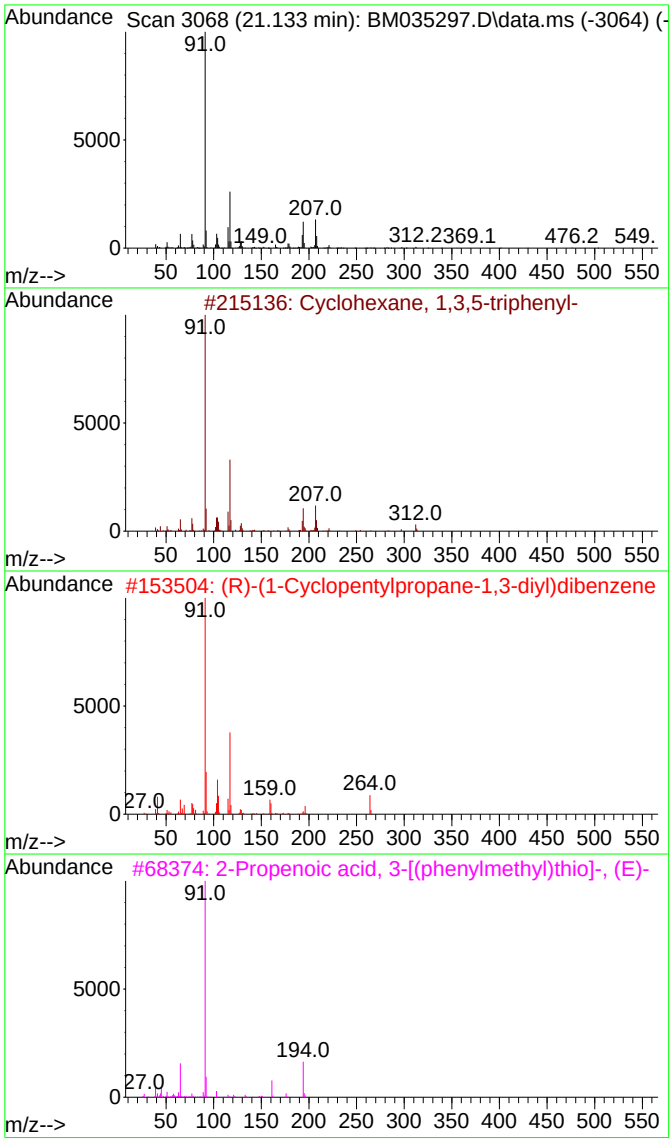
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

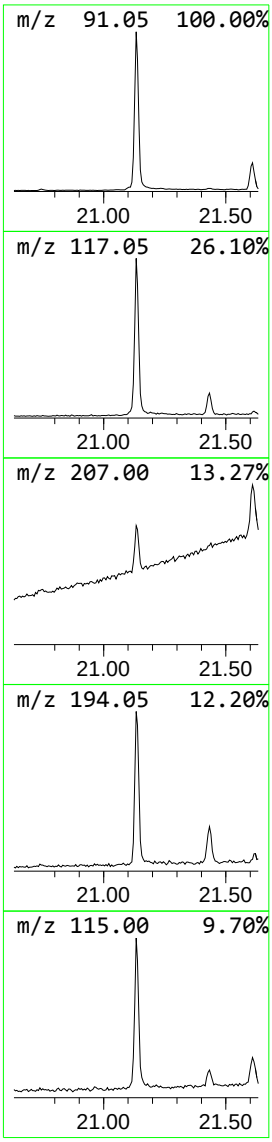
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclohexane, 1,3,5-triphenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	12.59 ng	1096660	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3,5-triphenyl-	312	C24H24	028336-57-4	86
2	(R)-(1-Cyclopentylpropane-1,3-di...	264	C20H24	1402851-74-4	38
3	2-Propenoic acid, 3-[(phenylmeth...	194	C10H10O2S	013831-01-1	25
4	Alpha-phenyl-alpha-tropylacetald...	378	C22H22N2O2S	022532-16-7	16
5	Benzyl phenyl sulfone	232	C13H12O2S	003112-88-7	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035297.D
Acq On : 27 May 2022 20:03
Operator : CG/JU
Sample : N2930-21
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P006-SS002-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

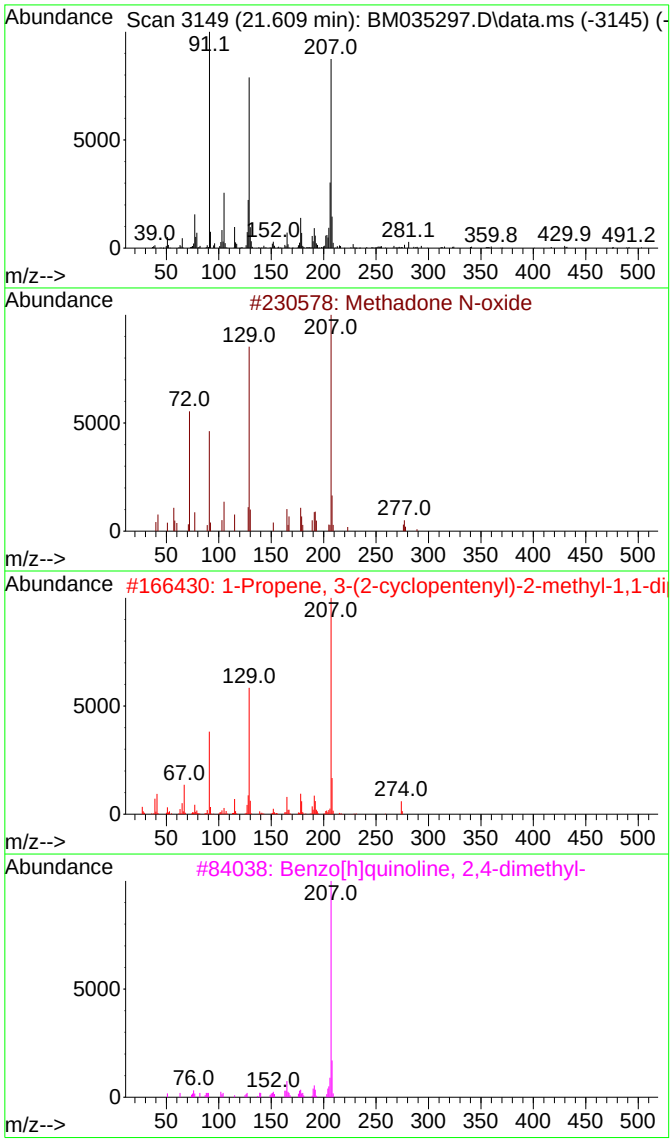
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

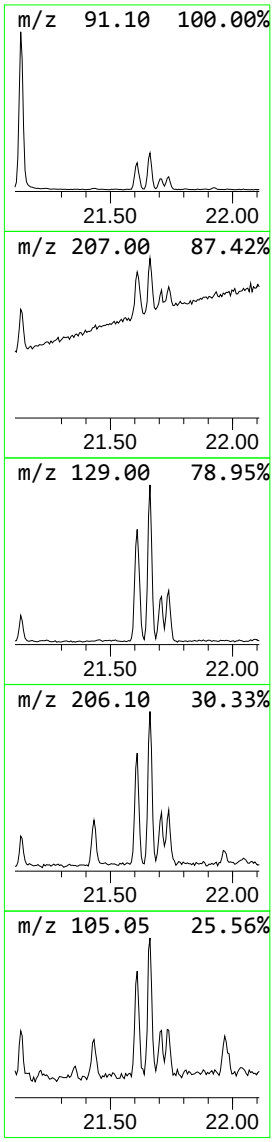
****

Peak Number 4 Methadone N-oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.609	3.61 ng	314451	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methadone N-oxide	325	C21H27NO2	1000120-80-7	72
2	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1010154-23-3	52
3	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	46
4	3-Methyl-2-phenylindole	207	C15H13N	010257-92-8	38
5	2-Methyl-7-phenylindole	207	C15H13N	001140-08-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035297.D
Acq On : 27 May 2022 20:03
Operator : CG/JU
Sample : N2930-21
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P006-SS002-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

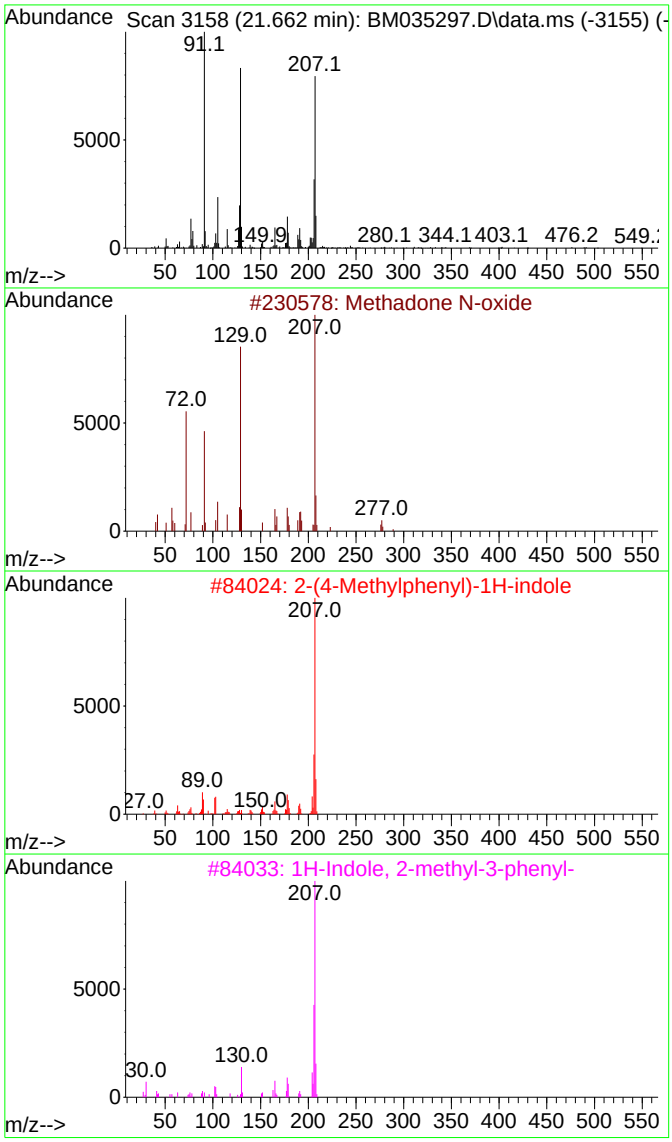
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

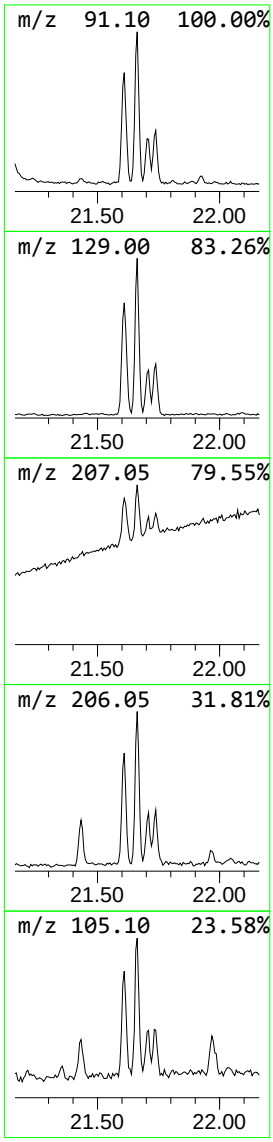
****

Peak Number 5 2-(4-Methylphenyl)-1H-indole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.662	3.04 ng	264342	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methadone N-oxide	325	C21H27NO2	1000120-80-7	80
2	2-(4-Methylphenyl)-1H-indole	207	C15H13N	055577-25-8	55
3	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	50
4	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	45
5	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035297.D
Acq On : 27 May 2022 20:03
Operator : CG/JU
Sample : N2930-21
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P006-SS002-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

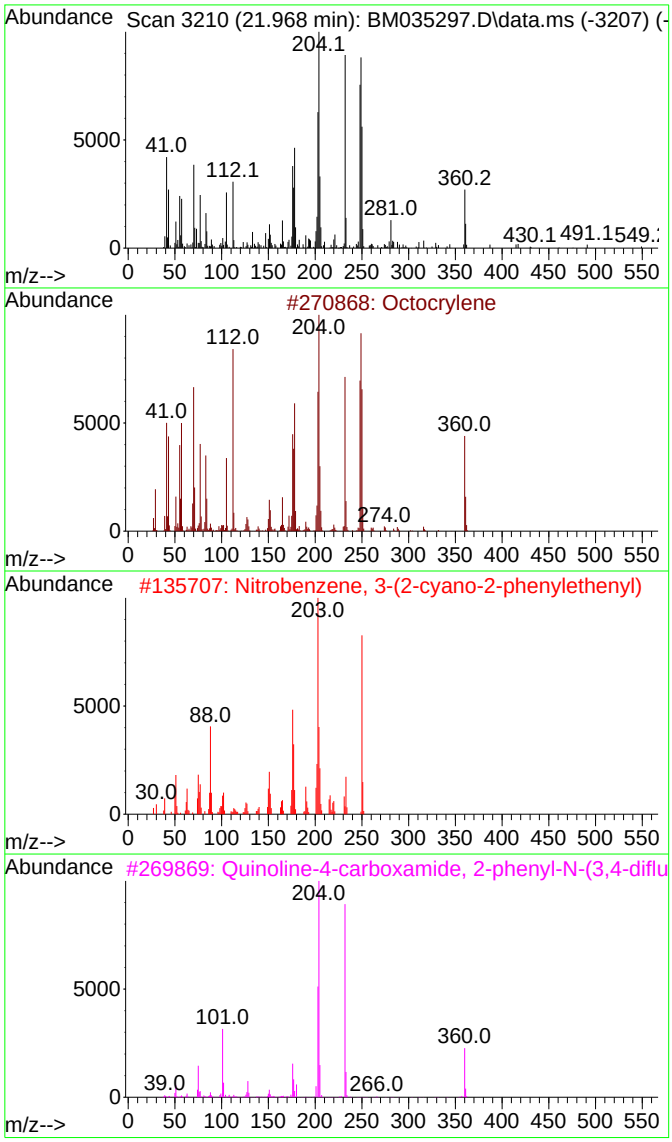
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

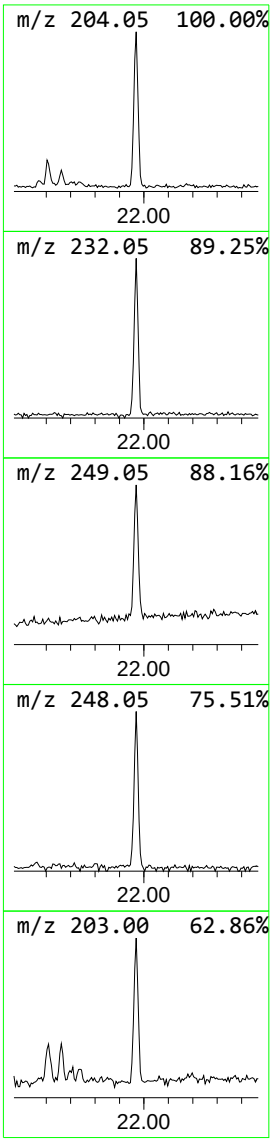
****

Peak Number 6 Octocrylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.968	2.01 ng	174961	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octocrylene	361	C24H27NO2	006197-30-4	70
2	Nitrobenzene, 3-(2-cyano-2-pheny...	250	C15H10N2O2	006720-37-2	53
3	Quinoline-4-carboxamide, 2-pheny...	360	C22H14F2N2O	303133-50-8	46
4	8-Phenylquinoline-6-carboxylic acid	249	C16H11NO2	035871-15-9	43
5	Benzene-1,4-diamine, N-(2-methyl...	249	C16H15N3	1000269-06-5	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052722\
Data File : BM035297.D
Acq On : 27 May 2022 20:03
Operator : CG/JU
Sample : N2930-21
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P006-SS002-2430-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052722.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
n-Hexadecanoic ...	18.157	6.5	ng	441420	4	17.257	1356810	20.0
Octadecanoic acid	19.433	4.5	ng	393733	5	21.433	1741760	20.0
Cyclohexane, 1,...	21.133	12.6	ng	1096660	5	21.433	1741760	20.0
Methadone N-oxide	21.609	3.6	ng	314451	5	21.433	1741760	20.0
2-(4-Methylphen...	21.662	3.0	ng	264342	5	21.433	1741760	20.0
Octocrylene	21.968	2.0	ng	174961	5	21.433	1741760	20.0