LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133654.D
Acq On : 08 Jun 2023 22:56
Operator : CG\JU
Sample : PB153207BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153207BL

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: BF133654.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.046	499	503	508	rBV	33061	38615	2.21%	0.293%
2	5.451	567	572	575	rBV	1843020	1700282	97.42%	12.920%
3	6.463	739	744	747	rBV	1794798	1691569	96.93%	12.854%
4	6.840	804	808	811	rBV	729207	596071	34.15%	4.529%
5	7.398	899	903	906	rBV	1238249	1011996	57.99%	7.690%
6	8.122	1022	1026	1029	rBV	925223	691557	39.63%	5.255%
7	9.198	1205	1209	1212	rBV	2154231	1745232	100.00%	13.261%
8	9.875	1321	1324	1328	rBV	767969	644932	36.95%	4.901%
9	10.592	1442	1446	1449	rBV	233458	195769	11.22%	1.488%
10	10.663	1454	1458	1462	rBV	1051649	935311	53.59%	7.107%
11	11.369	1574	1578	1581	rBV	697293	639356	36.63%	4.858%
12	11.892	1664	1667	1671	rBV2	50132	51381	2.94%	0.390%
13	12.580	1781	1784	1788	rVB	30655	25703	1.47%	0.195%
14	12.810	1818	1823	1825	rBV	26915	24692	1.41%	0.188%
15	12.957	1844	1848	1851	rBV	1775054	1521635	87.19%	11.562%
16	13.874	1999	2004	2015	rBV5	50169	151547	8.68%	1.152%
17	14.010	2023	2027	2031	rBV	517023	473604	27.14%	3.599%
18	14.480	2105	2107	2110	rBV2	27630	30659	1.76%	0.233%
19	14.645	2131	2135	2139	rBV	558214	545439	31.25%	4.145%
20	14.939	2182	2185	2188	rBV	40432	38880	2.23%	0.295%
21	15.127	2215	2217	2221	rVB2	45715	46753	2.68%	0.355%
22	15.480	2272	2277	2281	rBV	284242	359315	20.59%	2.730%

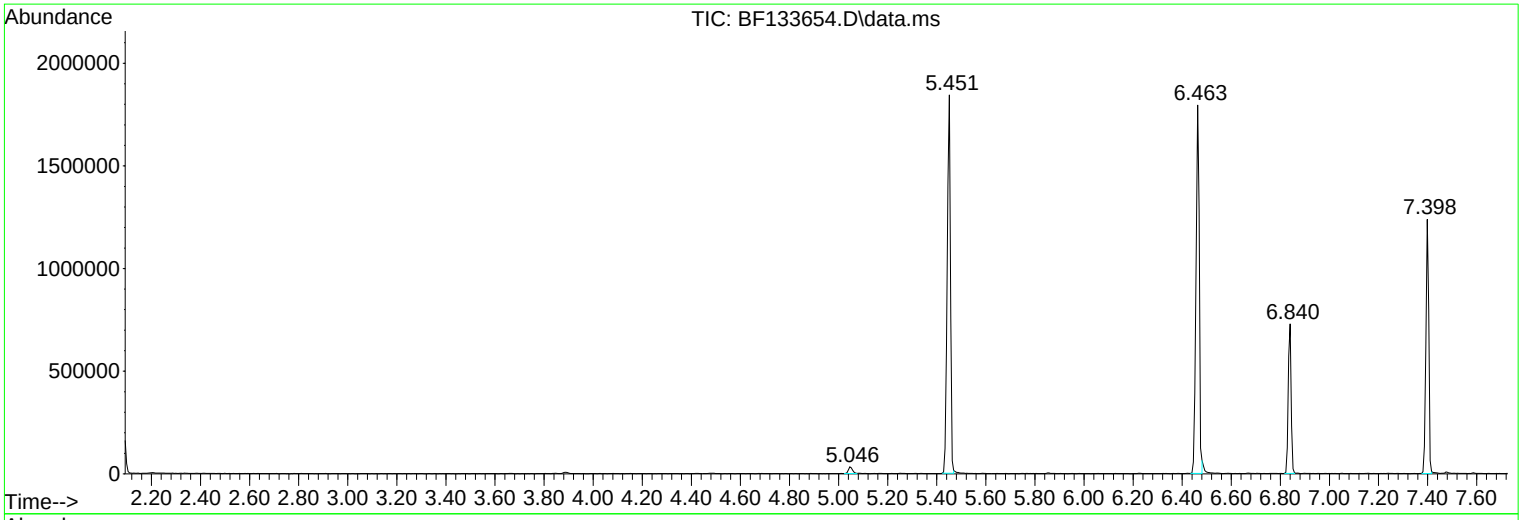
Sum of corrected areas: 13160298

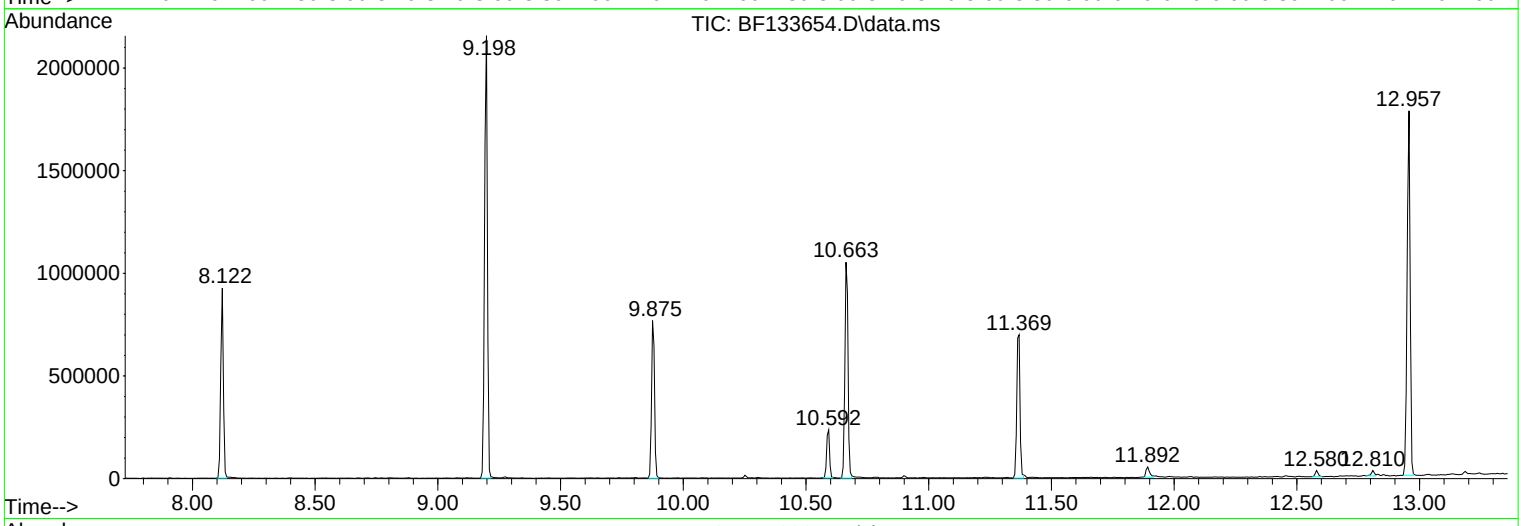
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133654.D
Acq On : 08 Jun 2023 22:56
Operator : CG\JU
Sample : PB153207BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

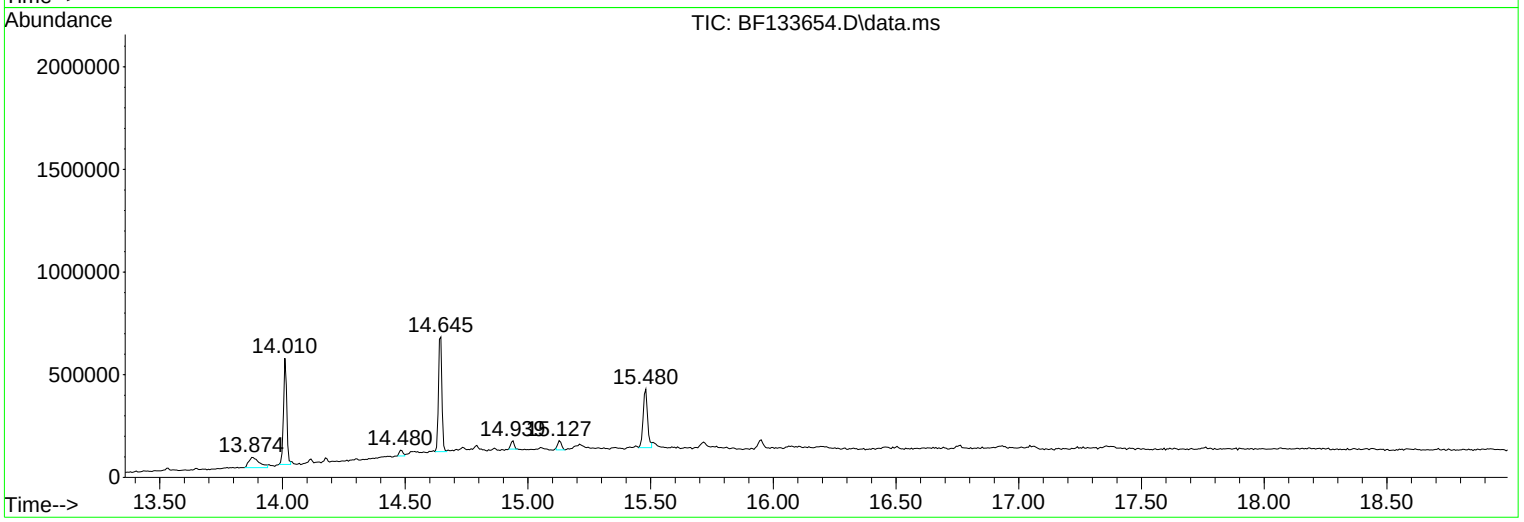
Instrument :
BNA_F
ClientSampleId :
PB153207BL

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\BF060823\
Data File : BF133654.D
Acq On : 08 Jun 2023 22:56
Operator : CG\JU
Sample : PB153207BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153207BL

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

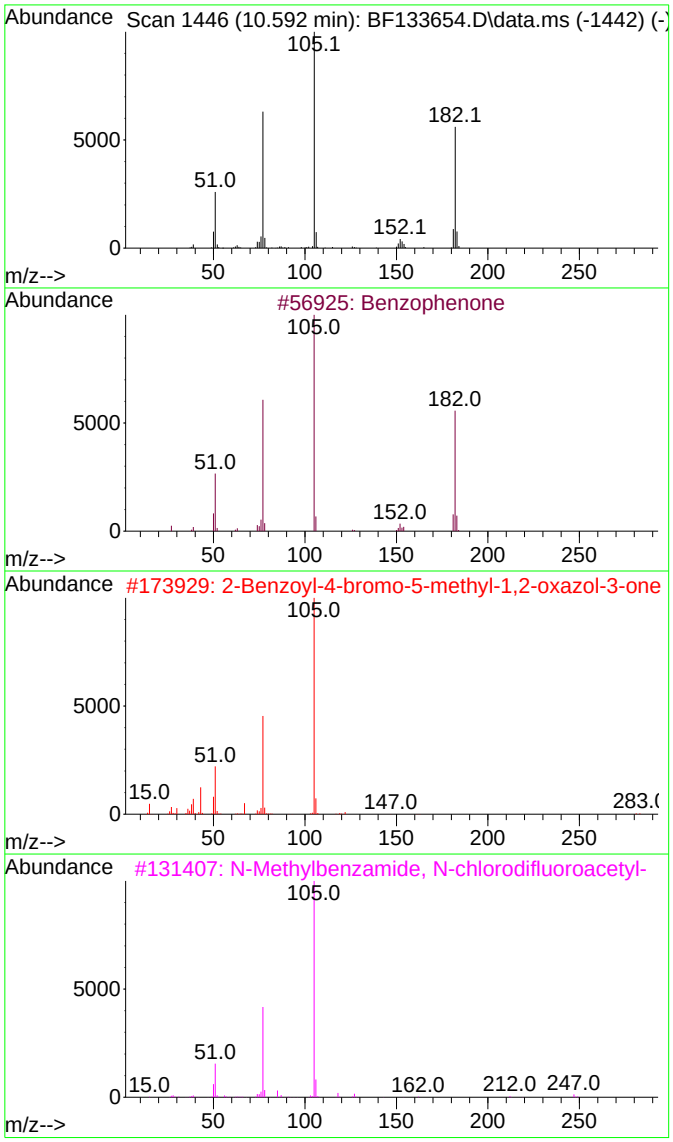
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

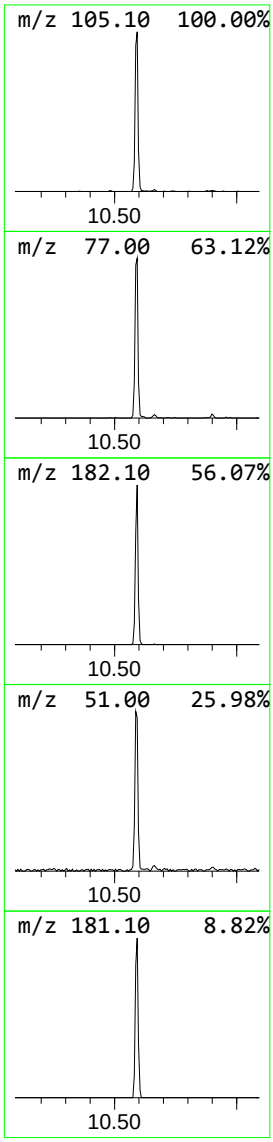
****

Peak Number 1 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.592	6.07 ng	195769	Acenaphthene-d10	9.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
3	N-Methylbenzamide, N-chlorodiflu...	247	C10H8ClF2NO2	1000446-98-2	47
4	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133654.D
Acq On : 08 Jun 2023 22:56
Operator : CG\JU
Sample : PB153207BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153207BL

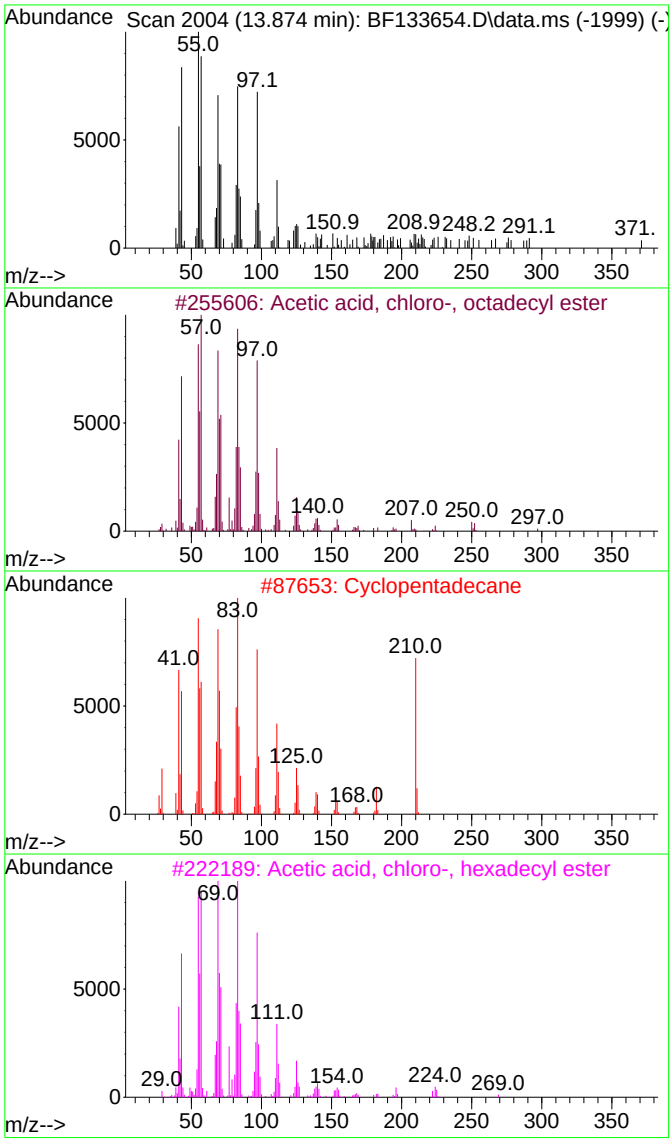
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

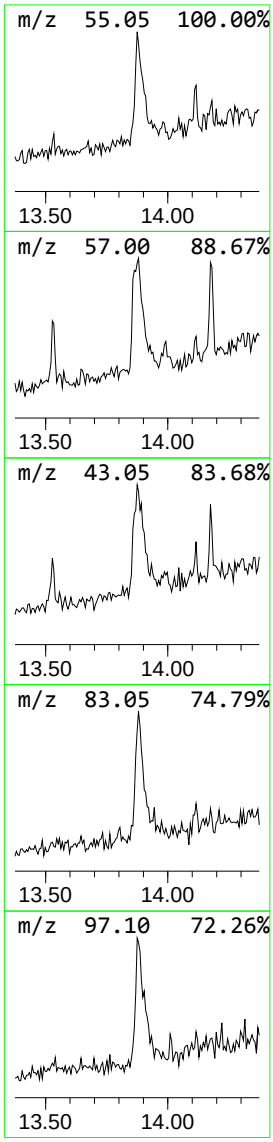
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Acetic acid, chloro-, octad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	6.40 ng	151547	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	95
2	Cyclopentadecane	210	C15H30	000295-48-7	95
3	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	94
4	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	94
5	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133654.D
Acq On : 08 Jun 2023 22:56
Operator : CG\JU
Sample : PB153207BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153207BL

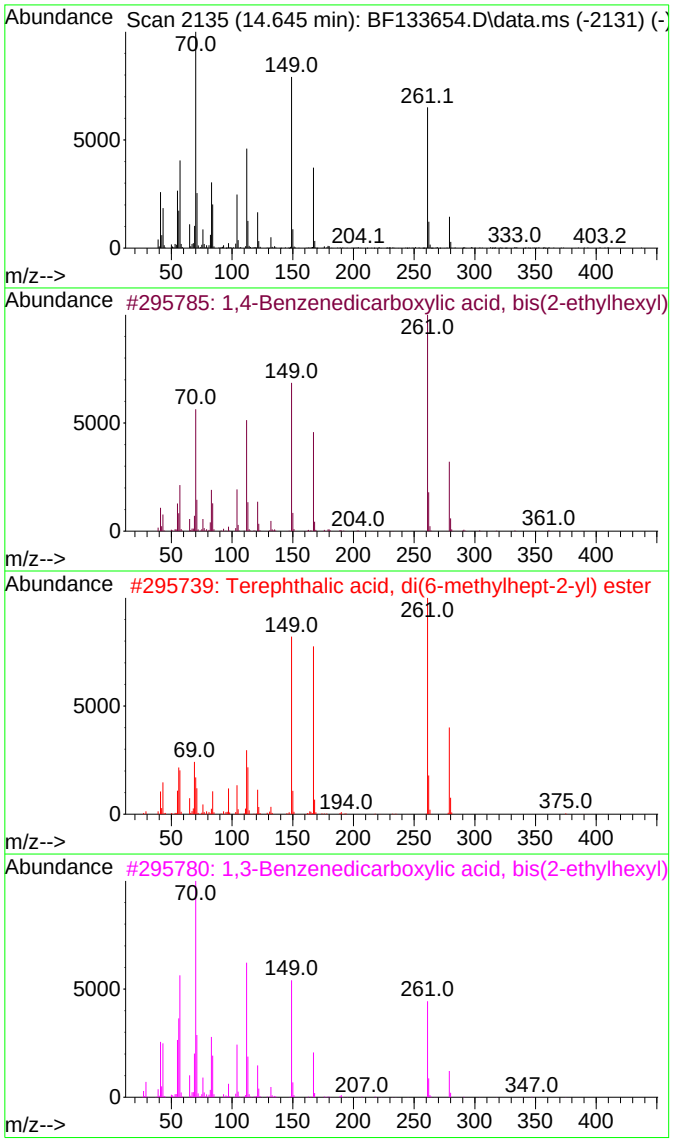
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

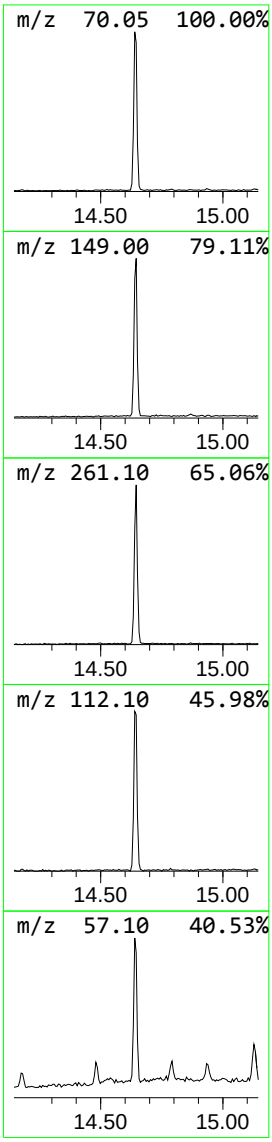
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1,4-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.645	23.03 ng	545439	Chrysene-d12	14.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	87
2	Terephthalic acid, di(6-methylhe...	390	C24H38O4	1000416-00-0	62
3	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	58
4	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	52
5	Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133654.D
Acq On : 08 Jun 2023 22:56
Operator : CG\JU
Sample : PB153207BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153207BL

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

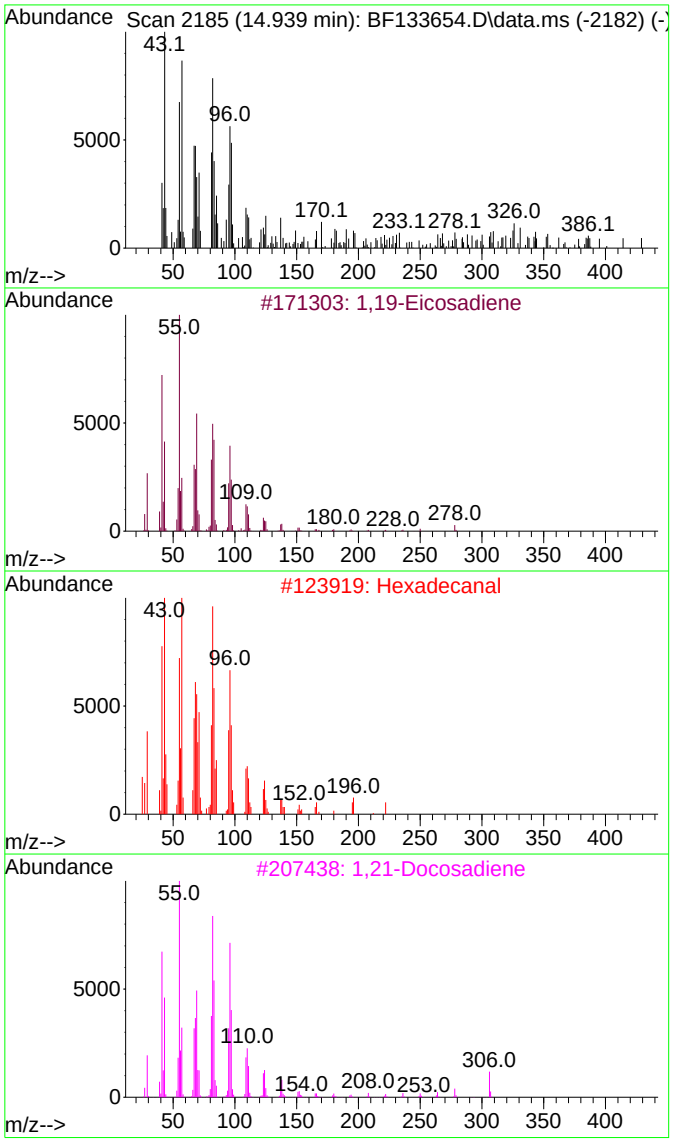
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

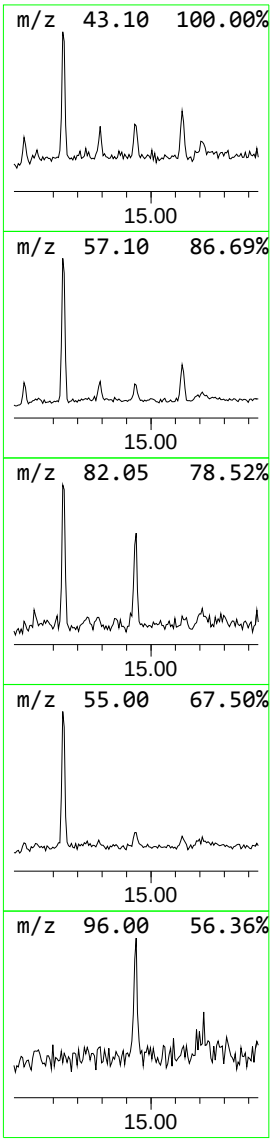
****

Peak Number 4 1,19-Eicosadiene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.939	2.16 ng	38880	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	83
2	Hexadecanal	240	C16H32O	000629-80-1	64
3	1,21-Docosadiene	306	C22H42	053057-53-7	64
4	Octadecanal	268	C18H36O	000638-66-4	64
5	Eicosanal-	296	C20H40O	002400-66-0	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133654.D
Acq On : 08 Jun 2023 22:56
Operator : CG\JU
Sample : PB153207BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153207BL

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

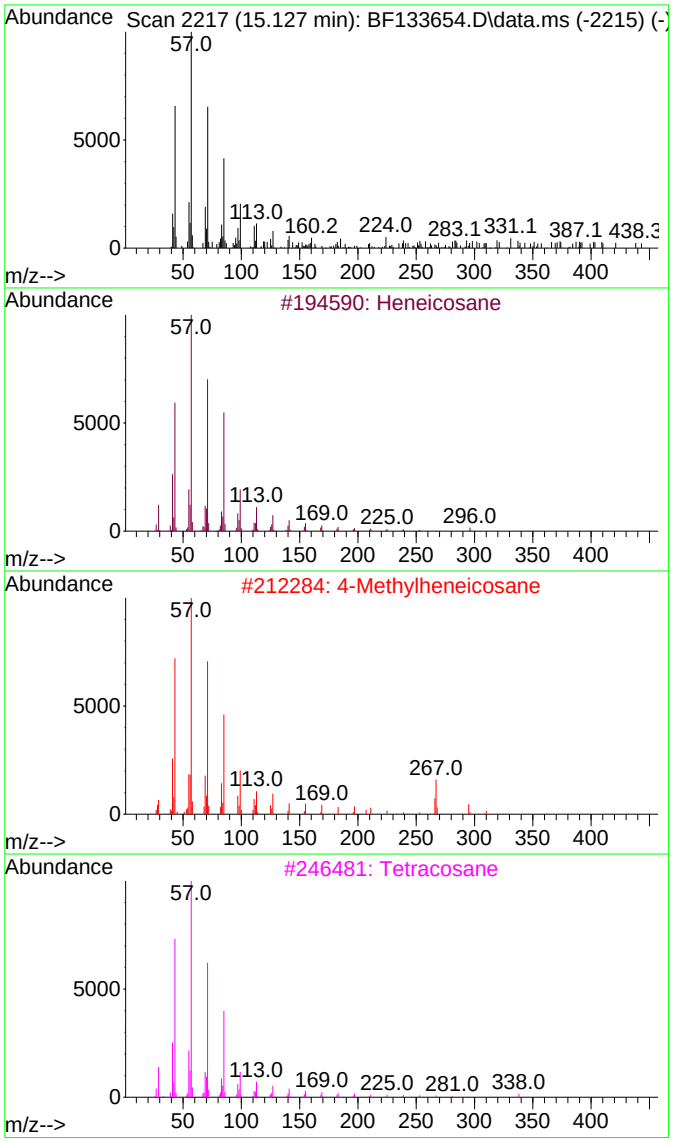
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

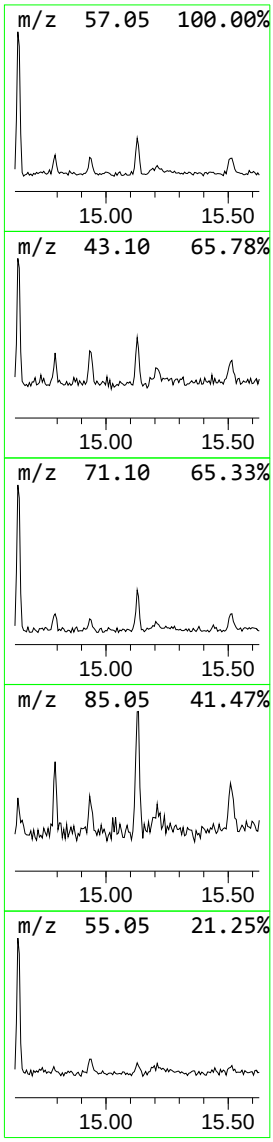
****

Peak Number 5 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	2.60 ng	46753	Perylene-d12	15.480

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	93
2	4-Methylheneicosane	310	C22H46	025117-29-7	93
3	Tetracosane	338	C24H50	000646-31-1	89
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	89
5	Tricosane, 2-methyl-	338	C24H50	001928-30-9	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060823\
Data File : BF133654.D
Acq On : 08 Jun 2023 22:56
Operator : CG\JU
Sample : PB153207BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB153207BL

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
Benzophenone	10.592	6.1	ng	195769	3	9.875	644932	20.0
Acetic acid, ch...	13.874	6.4	ng	151547	5	14.010	473604	20.0
1,4-Benzenedica...	14.645	23.0	ng	545439	5	14.010	473604	20.0
1,19-Eicosadiene	14.939	2.2	ng	38880	6	15.480	359315	20.0
Heneicosane	15.127	2.6	ng	46753	6	15.480	359315	20.0