LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120524\
Data File : BF140752.D
Acq On : 05 Dec 2024 16:53
Operator : RC/JU
Sample : P5096-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-A

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-BF112124.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140752.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	3	10	20	rVB	805852	1303132	50.40%	7.702%
2	2.258	23	28	39	rVB	28711	46458	1.80%	0.275%
3	5.099	505	511	526	rVB	159357	260851	10.09%	1.542%
4	5.504	575	580	606	rBV	1371510	1939342	75.01%	11.462%
5	6.516	746	752	778	rBV	1381892	2050577	79.31%	12.119%
6	6.869	807	812	817	rBV	322246	391999	15.16%	2.317%
7	7.434	902	908	918	rBV	995115	1333299	51.57%	7.880%
8	7.687	946	951	963	rBV	36080	62840	2.43%	0.371%
9	8.145	1024	1029	1043	rBV	383160	519315	20.09%	3.069%
10	9.222	1206	1212	1222	rBV	2022298	2585544	100.00%	15.281%
11	9.904	1323	1328	1342	rBV	462454	589009	22.78%	3.481%
12	10.622	1444	1450	1458	rBV	312006	409076	15.82%	2.418%
13	10.698	1458	1463	1477	rBV	1089221	1487531	57.53%	8.791%
14	10.928	1496	1502	1512	rVB	29386	44946	1.74%	0.266%
15	11.398	1576	1582	1590	rBV	411036	568210	21.98%	3.358%
16	11.928	1664	1672	1680	rBV4	27143	78965	3.05%	0.467%
17	12.616	1785	1789	1796	rVB	34804	44417	1.72%	0.263%
18	12.845	1823	1828	1842	rVB	32098	61446	2.38%	0.363%
19	12.980	1846	1851	1861	rBV	1426000	1869151	72.29%	11.047%
20	13.463	1927	1933	1943	rVB	85898	131531	5.09%	0.777%
21	13.880	1999	2004	2006	rBV3	21539	33163	1.28%	0.196%
22	13.927	2007	2012	2024	rVB3	35311	112103	4.34%	0.663%
23	14.057	2029	2034	2043	rVB	290810	419213	16.21%	2.478%
24	14.204	2055	2059	2075	rVB	33189	84655	3.27%	0.500%
25	15.145	2214	2219	2223	rBV	19167	39459	1.53%	0.233%
26	15.580	2287	2293	2304	rBV	266588	454081	17.56%	2.684%

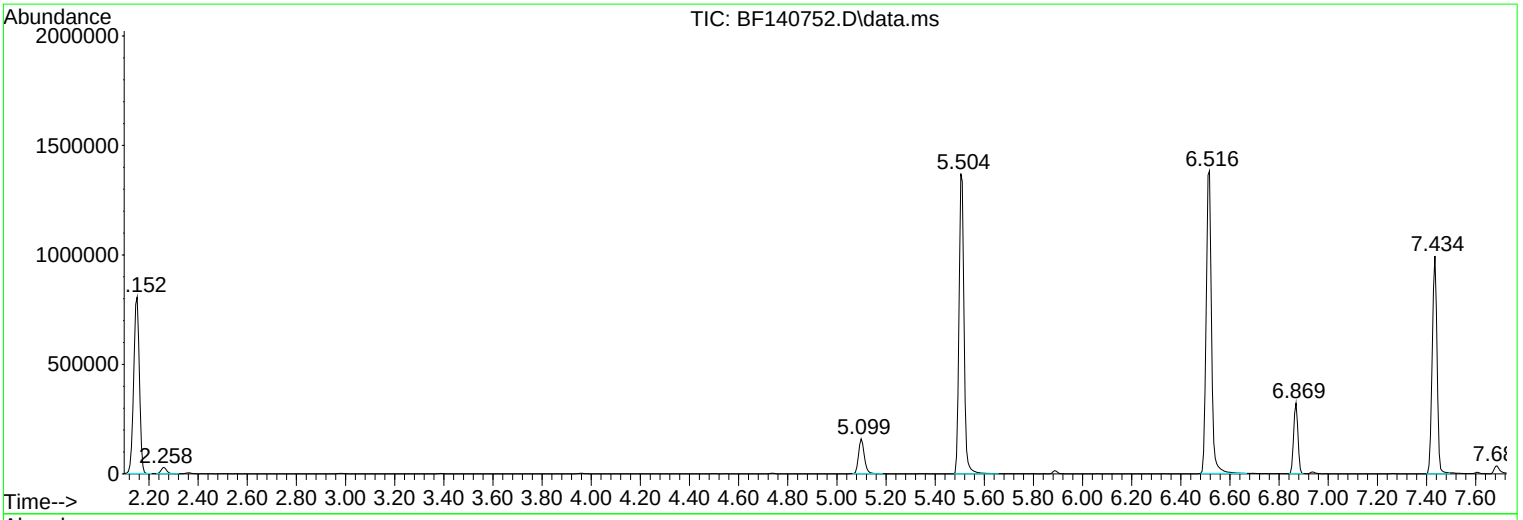
Sum of corrected areas: 16920313

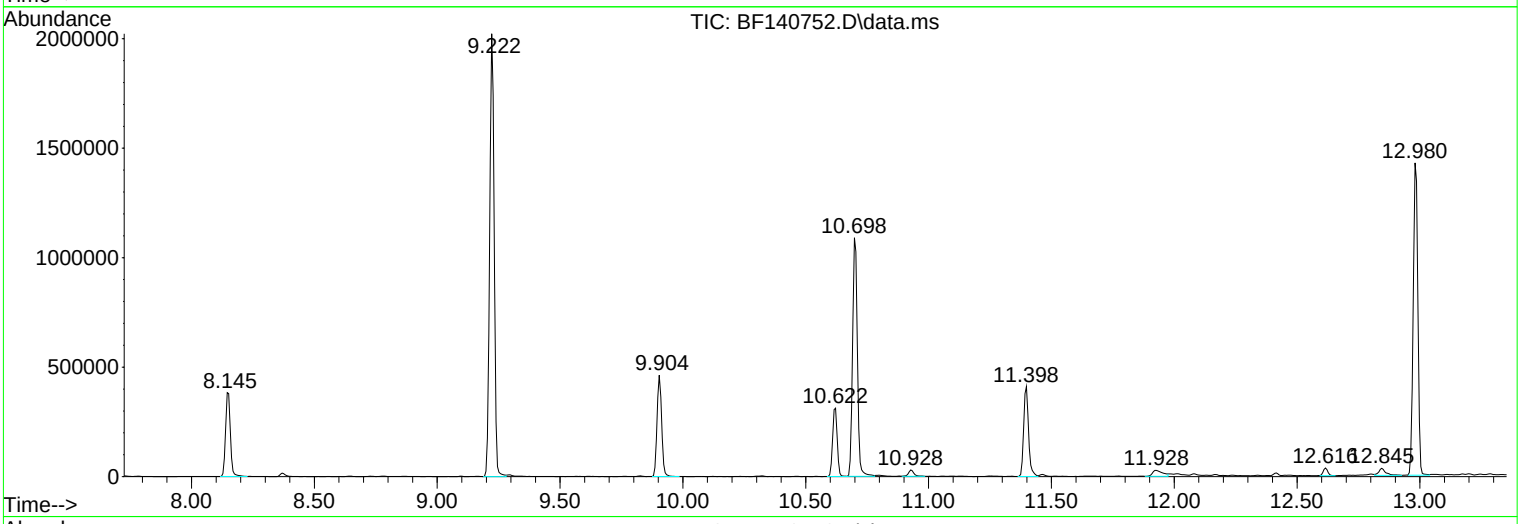
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120524\
Data File : BF140752.D
Acq On : 05 Dec 2024 16:53
Operator : RC/JU
Sample : P5096-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

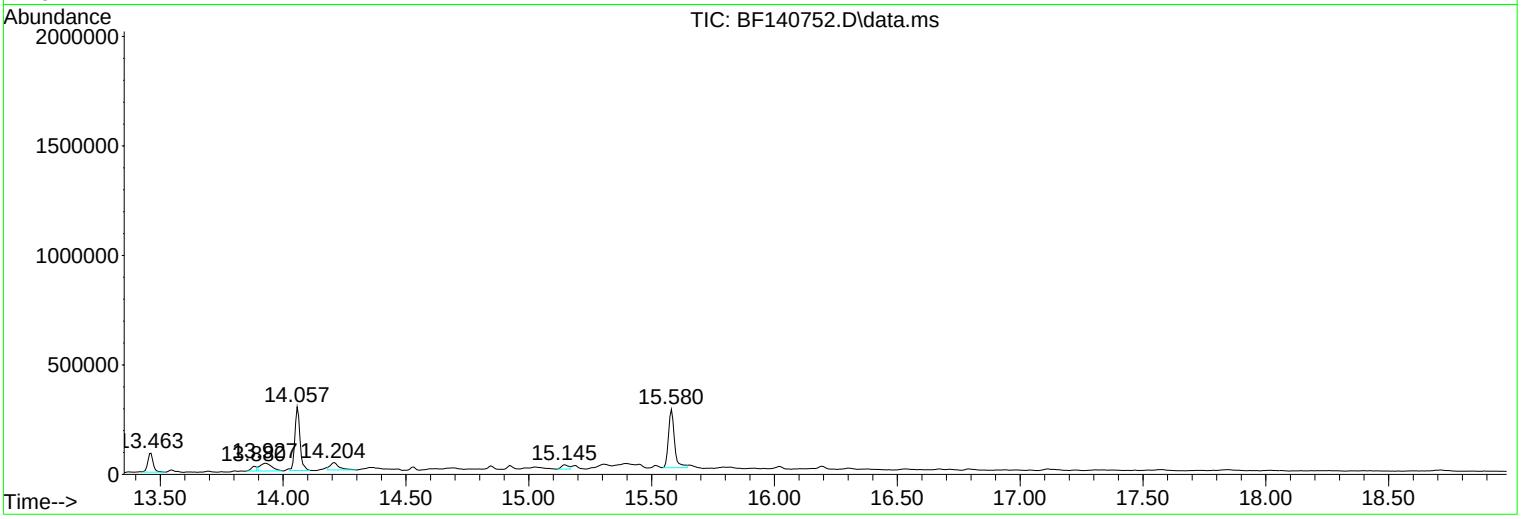
Instrument :
BNA_F
ClientSampleId :
MH-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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\BF120524\
Data File : BF140752.D
Acq On : 05 Dec 2024 16:53
Operator : RC/JU
Sample : P5096-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

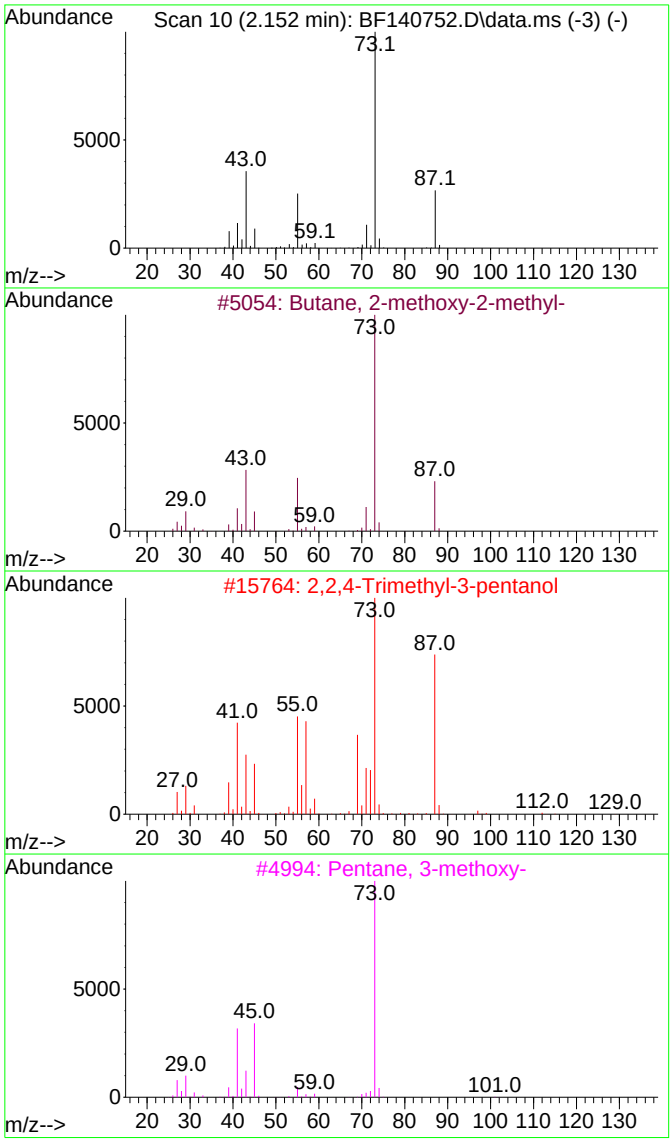
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

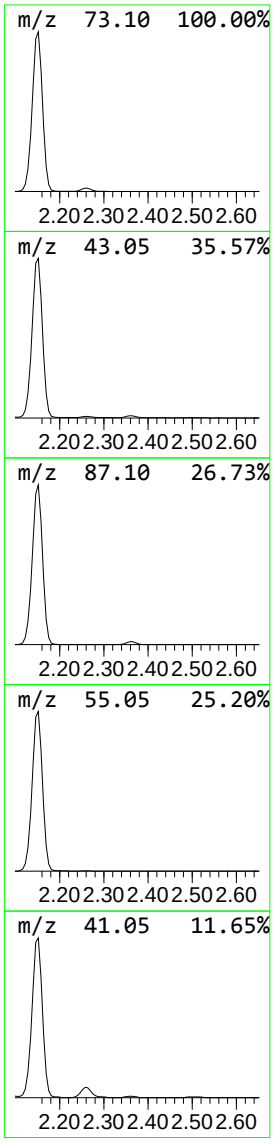
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	66.49 ng	1303130	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120524\
Data File : BF140752.D
Acq On : 05 Dec 2024 16:53
Operator : RC/JU
Sample : P5096-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

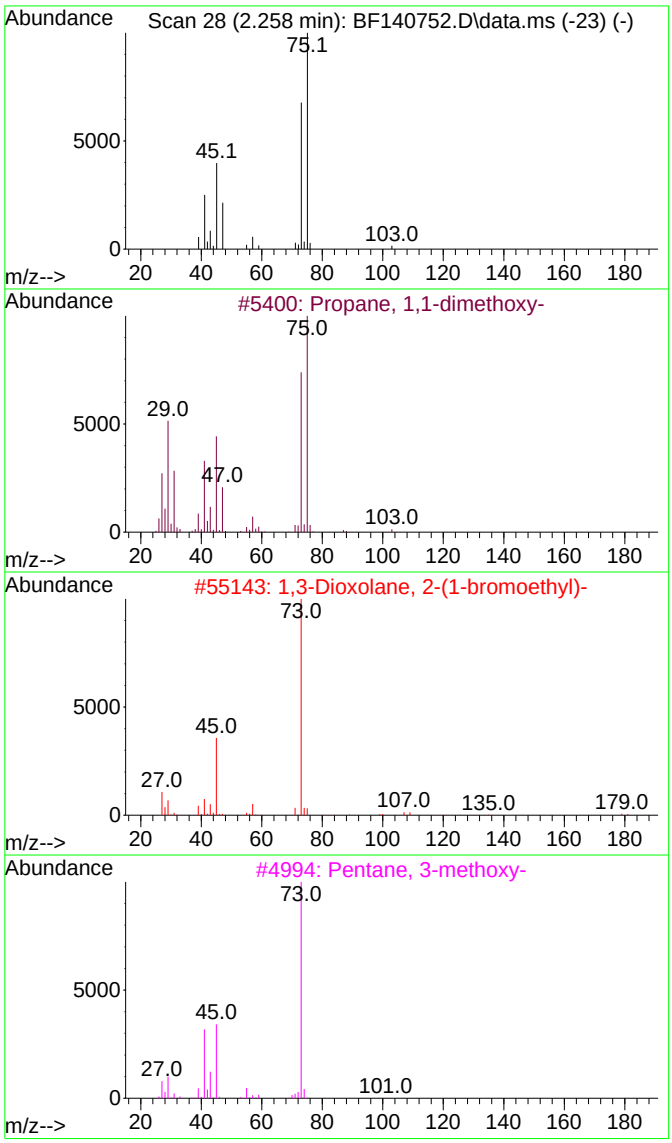
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

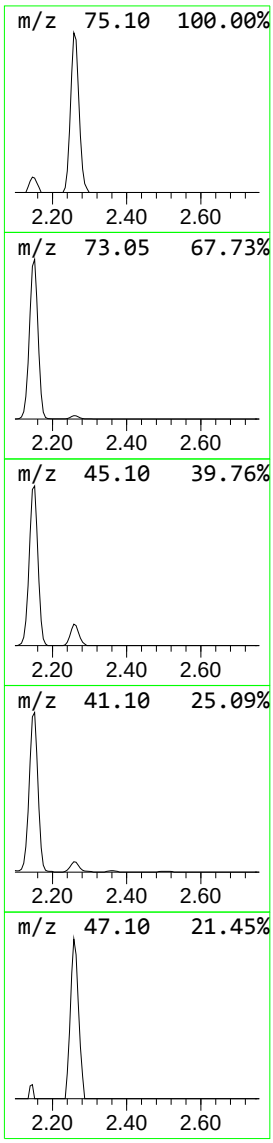
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.258	2.37 ng	46458	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	22
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
5	Ethane, 2-chloro-1,1-dimethoxy-	124	C4H9ClO2	000097-97-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120524\
Data File : BF140752.D
Acq On : 05 Dec 2024 16:53
Operator : RC/JU
Sample : P5096-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-A

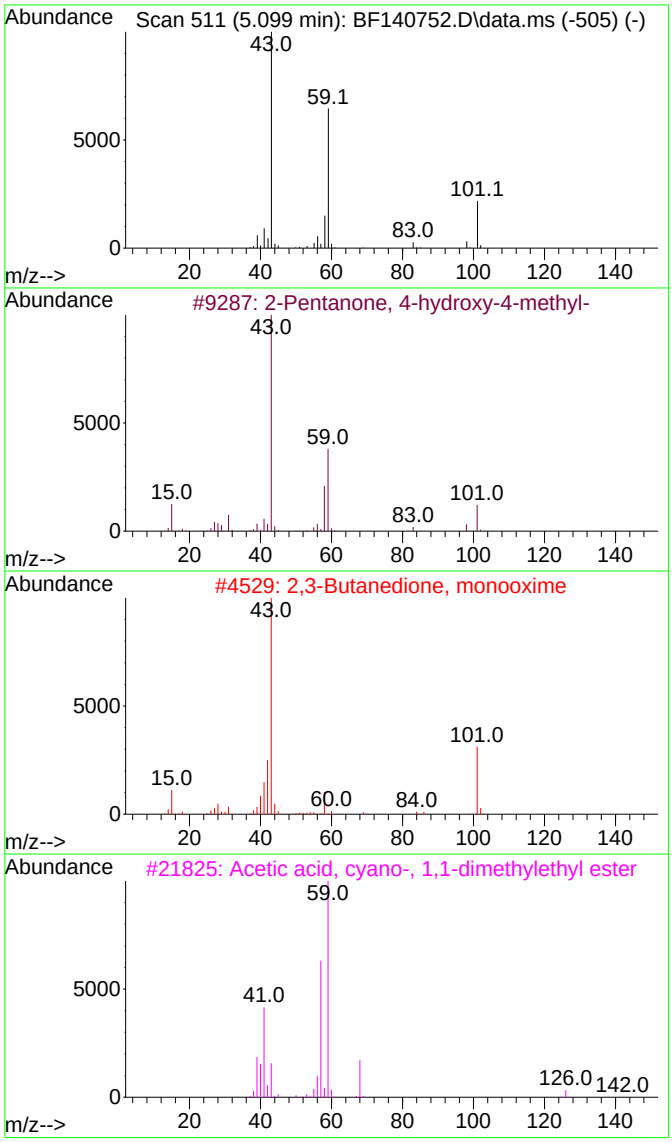
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

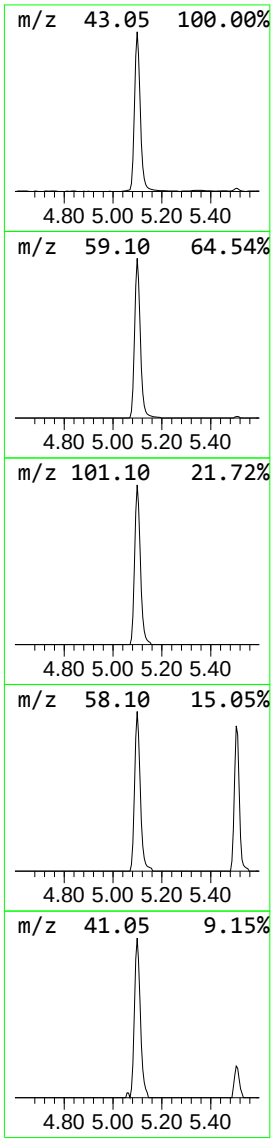
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.099	13.31 ng	260851	1,4-Dichlorobenzene-d4	6.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120524\
Data File : BF140752.D
Acq On : 05 Dec 2024 16:53
Operator : RC/JU
Sample : P5096-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

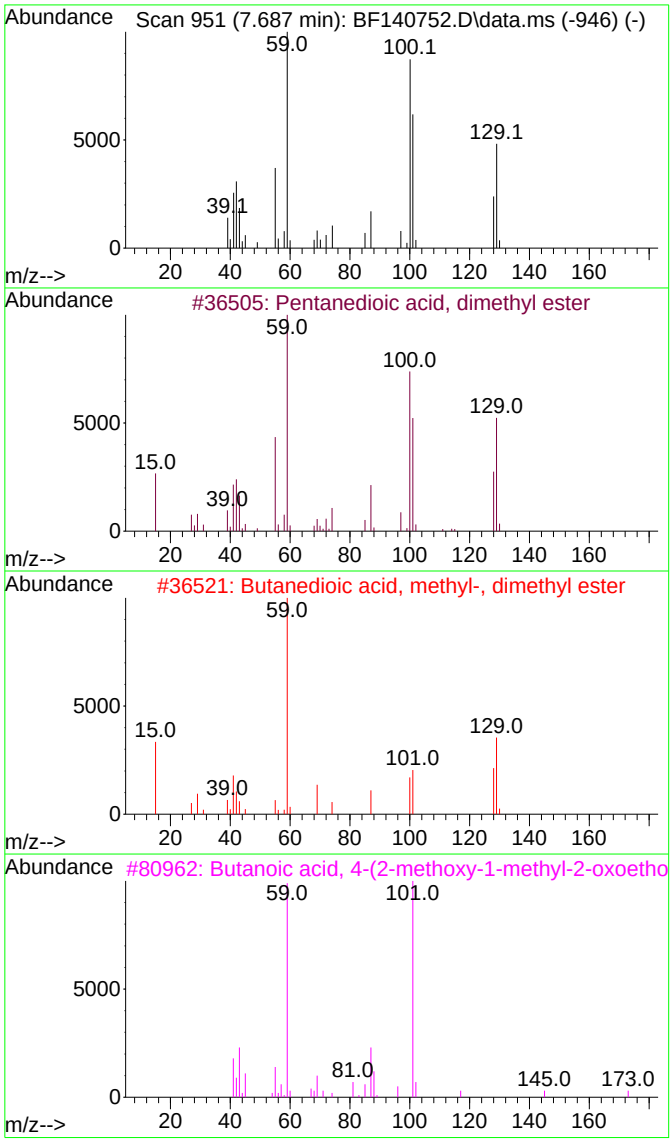
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

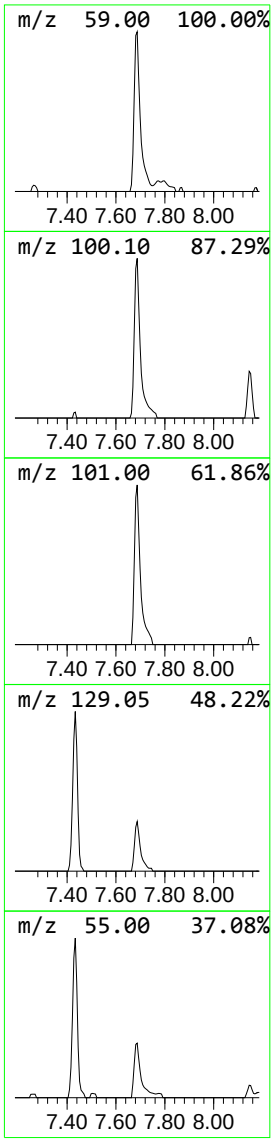
****

Peak Number 4 Pentanedioic acid, dimethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.687	2.42 ng	62840	Naphthalene-d8	8.151

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	91
2	Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	47
3	Butanoic acid, 4-(2-methoxy-1-me...	204	C9H16O5	054966-46-0	25
4	Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	25
5	1,4-Di-O-acetyl-2,5-di-O-methyl-...	262	C12H22O6	1000101-82-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120524\
Data File : BF140752.D
Acq On : 05 Dec 2024 16:53
Operator : RC/JU
Sample : P5096-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

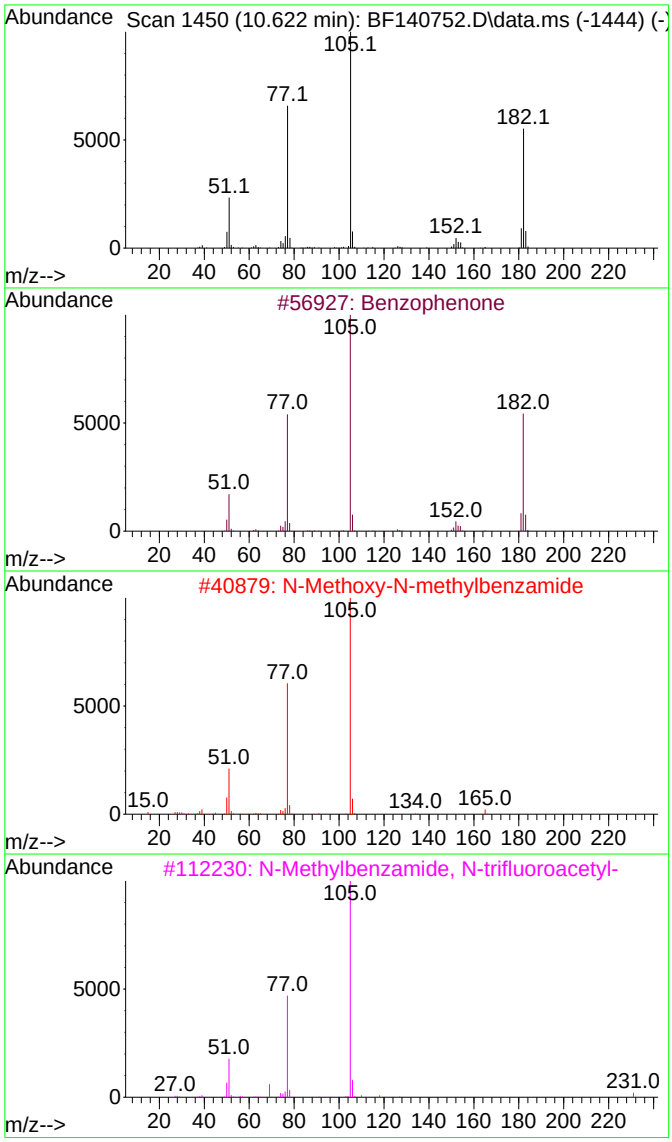
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

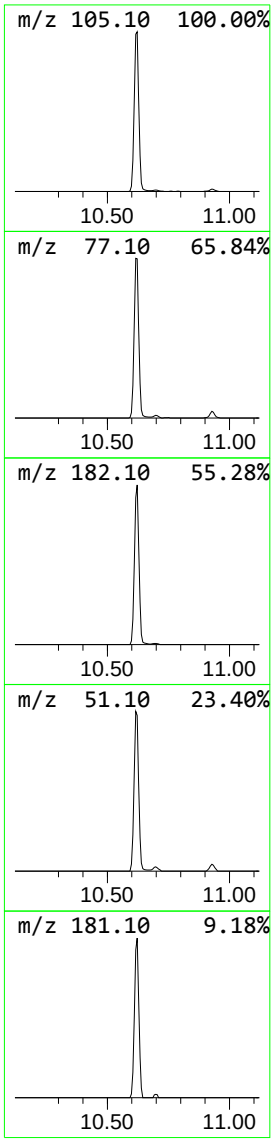
****

Peak Number 5 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.622	13.89 ng	409076	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
3	N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
4	N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	47
5	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120524\
Data File : BF140752.D
Acq On : 05 Dec 2024 16:53
Operator : RC/JU
Sample : P5096-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

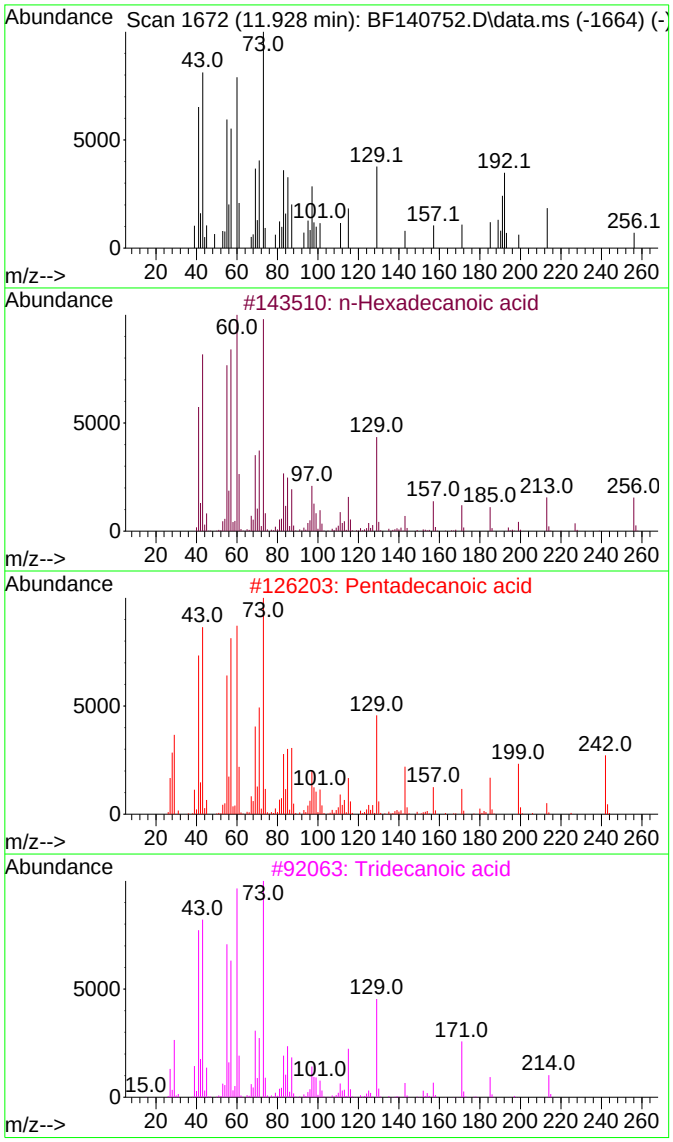
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

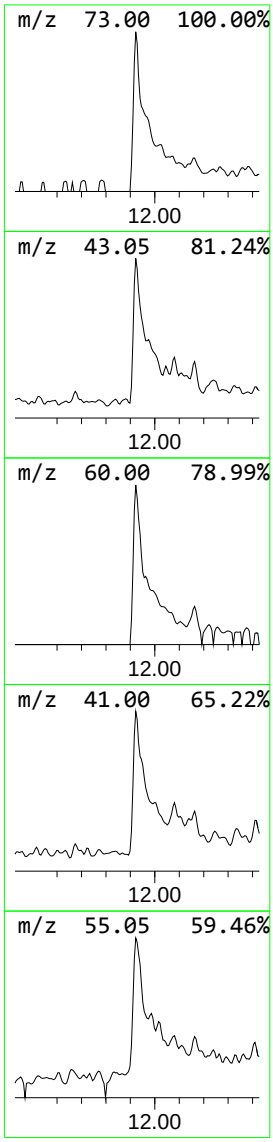
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	2.78 ng	78965	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120524\
Data File : BF140752.D
Acq On : 05 Dec 2024 16:53
Operator : RC/JU
Sample : P5096-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

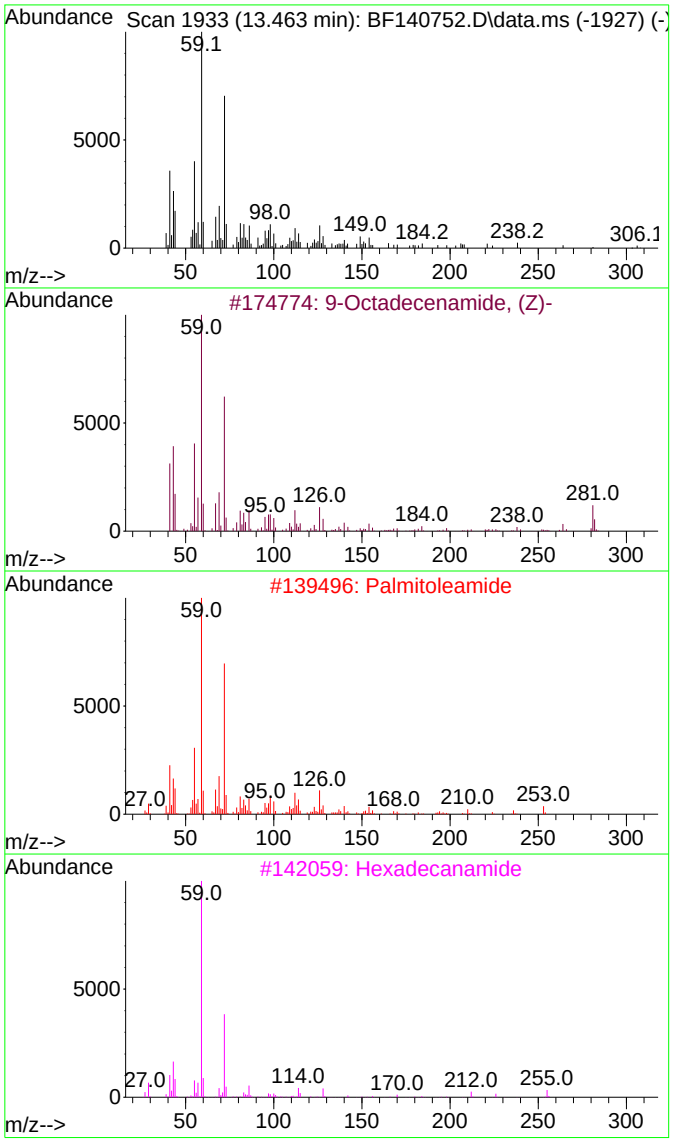
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

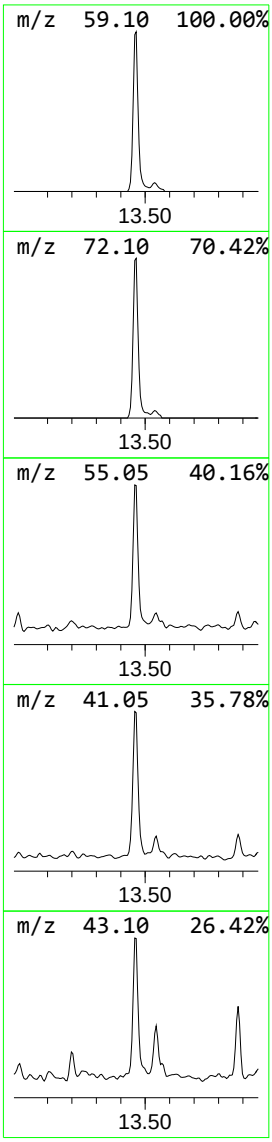
****

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.463	6.28 ng	131531	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2	Palmitoleamide	253	C16H31NO	106010-22-4	83
3	Hexadecanamide	255	C16H33NO	000629-54-9	64
4	Octadecanamide	283	C18H37NO	000124-26-5	58
5	Tetradecanamide	227	C14H29NO	000638-58-4	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120524\
Data File : BF140752.D
Acq On : 05 Dec 2024 16:53
Operator : RC/JU
Sample : P5096-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

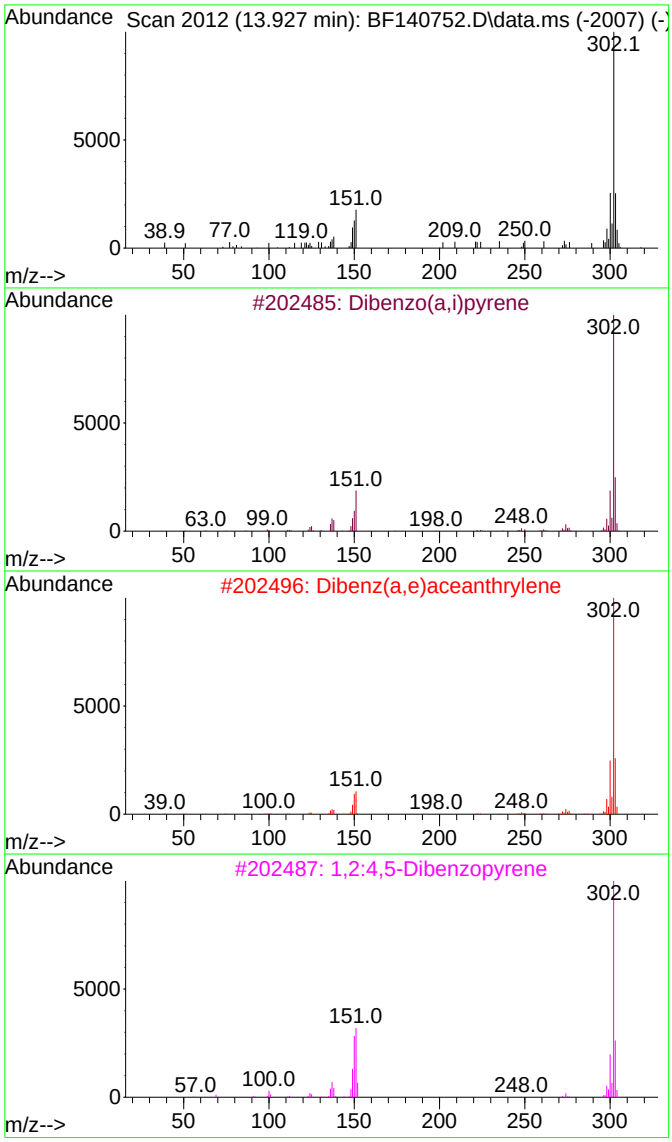
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

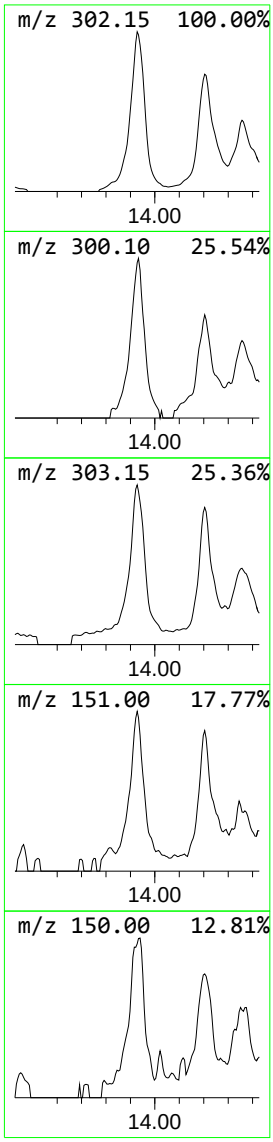
****

Peak Number 9 Dibenzo(a,i)pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	5.35 ng	112103	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo(a,i)pyrene	302	C24H14	000189-55-9	90
2	Dibenz(a,e)aceanthrylene	302	C24H14	005385-75-1	90
3	1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	90
4	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	81
5	1,2,9,10-Dibenzopyrene	302	C24H14	000191-30-0	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120524\
Data File : BF140752.D
Acq On : 05 Dec 2024 16:53
Operator : RC/JU
Sample : P5096-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

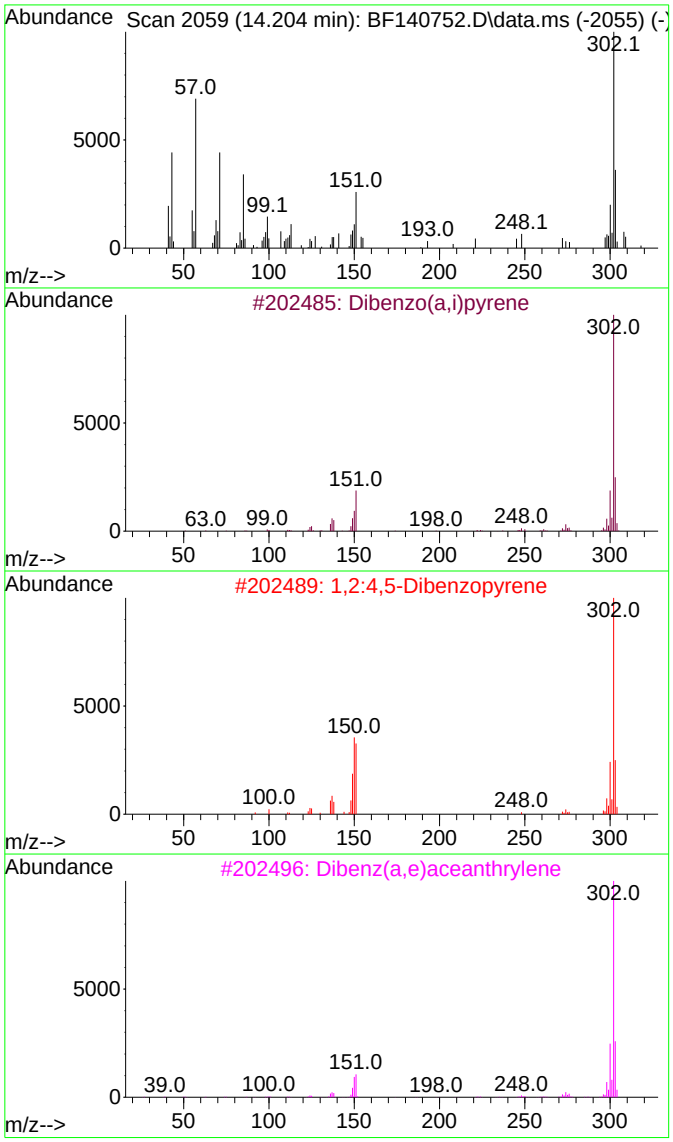
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

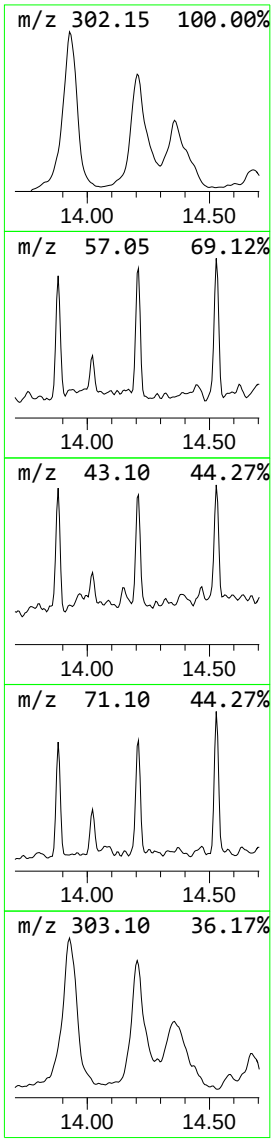
****

Peak Number 10 1,2:4,5-Dibenzopyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.204	4.04 ng	84655	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo(a,i)pyrene	302	C24H14	000189-55-9	76
2	1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	68
3	Dibenz(a,e)aceanthrylene	302	C24H14	005385-75-1	62
4	3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	60
5	1,2,9,10-Dibenzopyrene	302	C24H14	000191-30-0	55





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120524\
Data File : BF140752.D
Acq On : 05 Dec 2024 16:53
Operator : RC/JU
Sample : P5096-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112124.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
Butane, 2-metho...	2.152	66.5	ng	1303130	1	6.869	391999	20.0
Propane, 1,1-di...	2.258	2.4	ng	46458	1	6.869	391999	20.0
2-Pentanone, 4-...	5.099	13.3	ng	260851	1	6.869	391999	20.0
Pentanedioic ac...	7.687	2.4	ng	62840	2	8.151	519315	20.0
Benzophenone	10.622	13.9	ng	409076	3	9.904	589009	20.0
n-Hexadecanoic ...	11.928	2.8	ng	78965	4	11.398	568210	20.0
9-Octadecenamid...	13.463	6.3	ng	131531	5	14.057	419213	20.0
Dibenzo(a,i)pyrene	13.927	5.3	ng	112103	5	14.057	419213	20.0
1,2:4,5-Dibenzo...	14.204	4.0	ng	84655	5	14.057	419213	20.0