LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123486.D
Acq On : 26 Mar 2021 15:01
Operator : JU/CG
Sample : M1770-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-104D

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-BF032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123486.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.251	20	28	33	rVB	3427168	4531846	54.77%	8.857%
2	2.351	41	45	54	rVB	228264	294724	3.56%	0.576%
3	5.122	508	516	522	rBV	76386	108010	1.31%	0.211%
4	5.522	579	584	587	rBV	3623230	3615095	43.69%	7.065%
5	6.516	748	753	765	rBV	2997740	2846341	34.40%	5.563%
6	6.898	814	818	821	rBV	1822959	1444009	17.45%	2.822%
7	7.463	908	914	917	rBV	4653322	4879260	58.97%	9.536%
8	8.186	1028	1037	1040	rBV	1901229	1902515	22.99%	3.718%
9	9.263	1214	1220	1223	rBV	7971454	8274638	100.00%	16.172%
10	9.651	1283	1286	1290	rBV	133293	112001	1.35%	0.219%
11	9.945	1331	1336	1339	rVB	2344430	2156477	26.06%	4.215%
12	10.733	1463	1470	1473	rBV	5490683	5624736	67.98%	10.993%
13	11.433	1584	1589	1592	rBV	2600998	2116380	25.58%	4.136%
14	11.957	1673	1678	1693	rBV	589402	720768	8.71%	1.409%
15	12.745	1807	1812	1819	rBV2	81496	99616	1.20%	0.195%
16	13.027	1854	1860	1863	rBV	7969310	8110998	98.02%	15.852%
17	13.874	1998	2004	2007	rBV	91756	133933	1.62%	0.262%
18	13.915	2007	2011	2012	rVV	127390	135040	1.63%	0.264%
19	13.945	2012	2016	2029	rVB	677086	1145274	13.84%	2.238%
20	14.080	2034	2039	2042	rBV	1772831	1591434	19.23%	3.110%
21	14.557	2111	2120	2122	rBV2	65752	112777	1.36%	0.220%
22	15.580	2288	2294	2299	rBV	958110	1211911	14.65%	2.369%

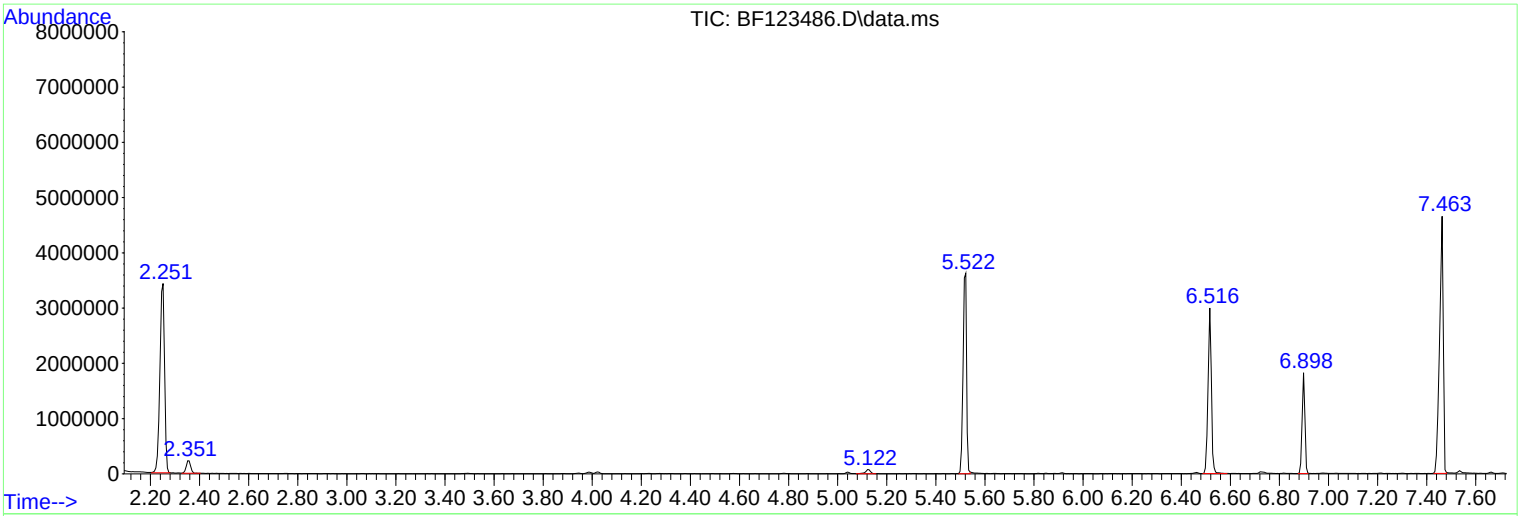
Sum of corrected areas: 51167783

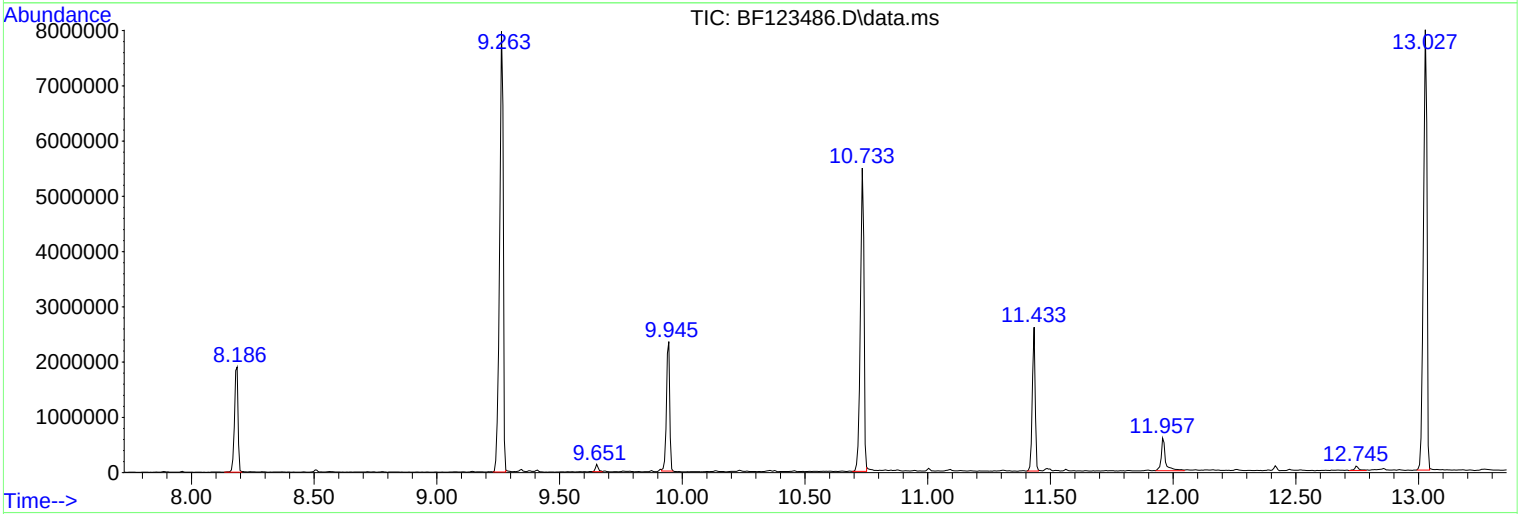
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123486.D
Acq On : 26 Mar 2021 15:01
Operator : JU/CG
Sample : M1770-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

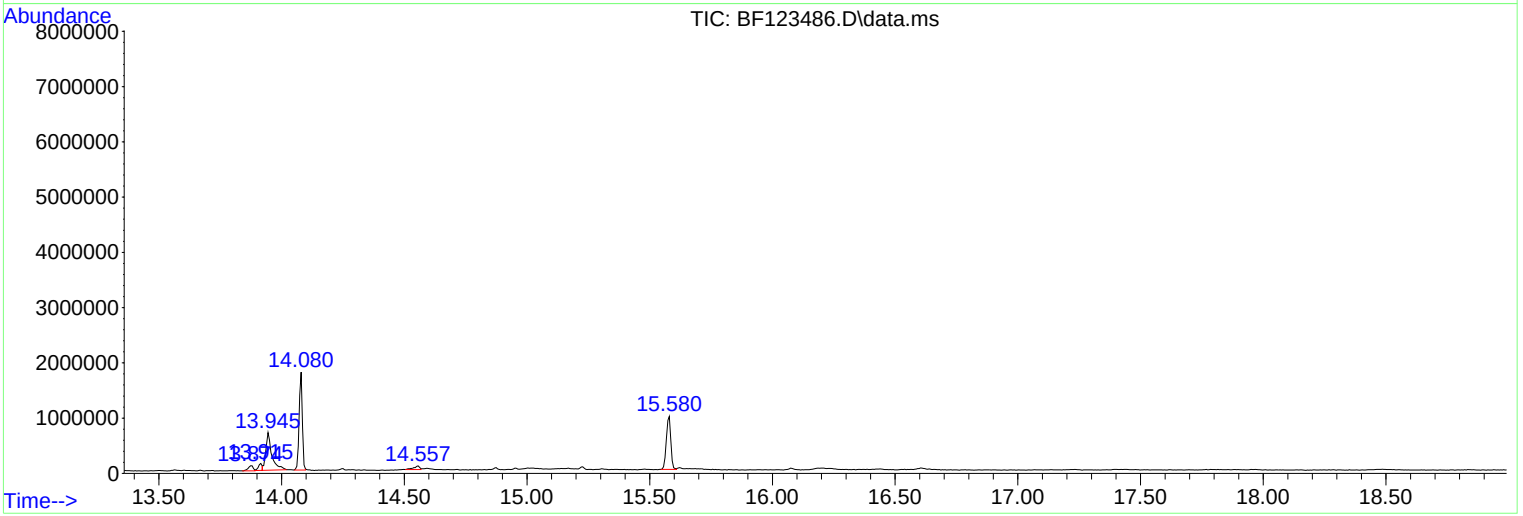
Instrument :
BNA_F
ClientSampleId :
MW-104D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123486.D
Acq On : 26 Mar 2021 15:01
Operator : JU/CG
Sample : M1770-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-104D

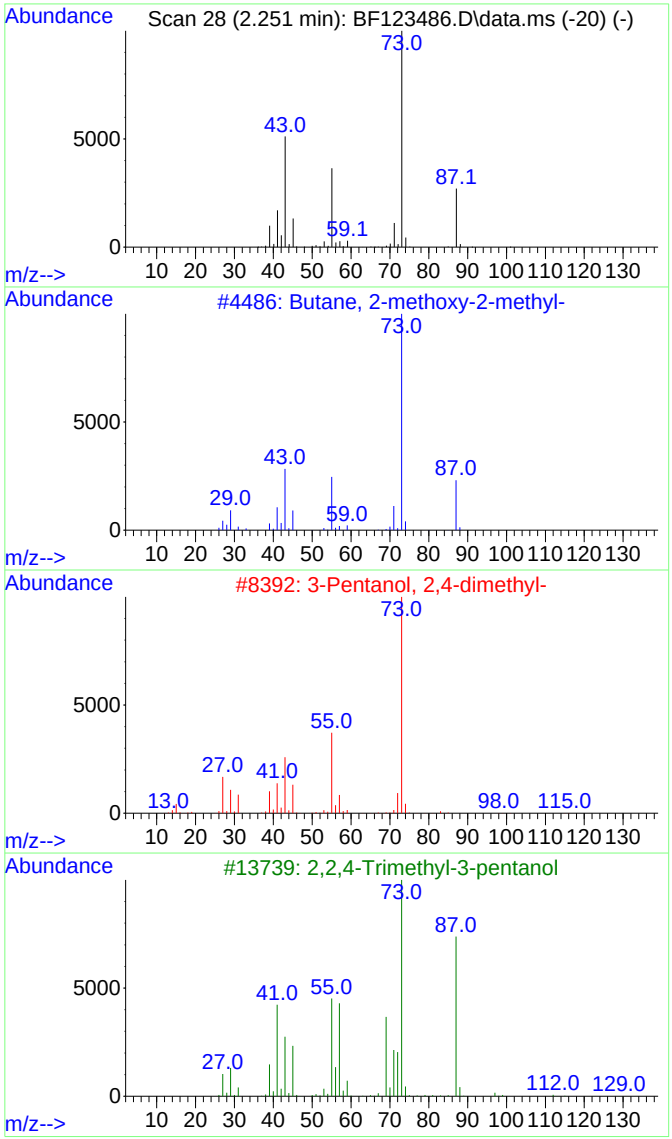
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

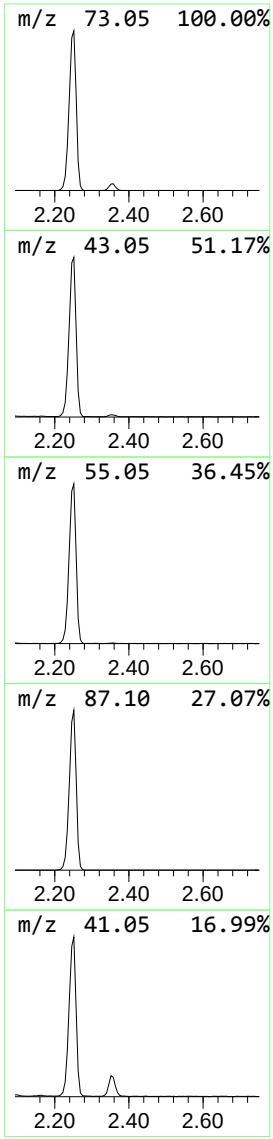
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.251	62.77 ng	4531850	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123486.D
Acq On : 26 Mar 2021 15:01
Operator : JU/CG
Sample : M1770-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-104D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

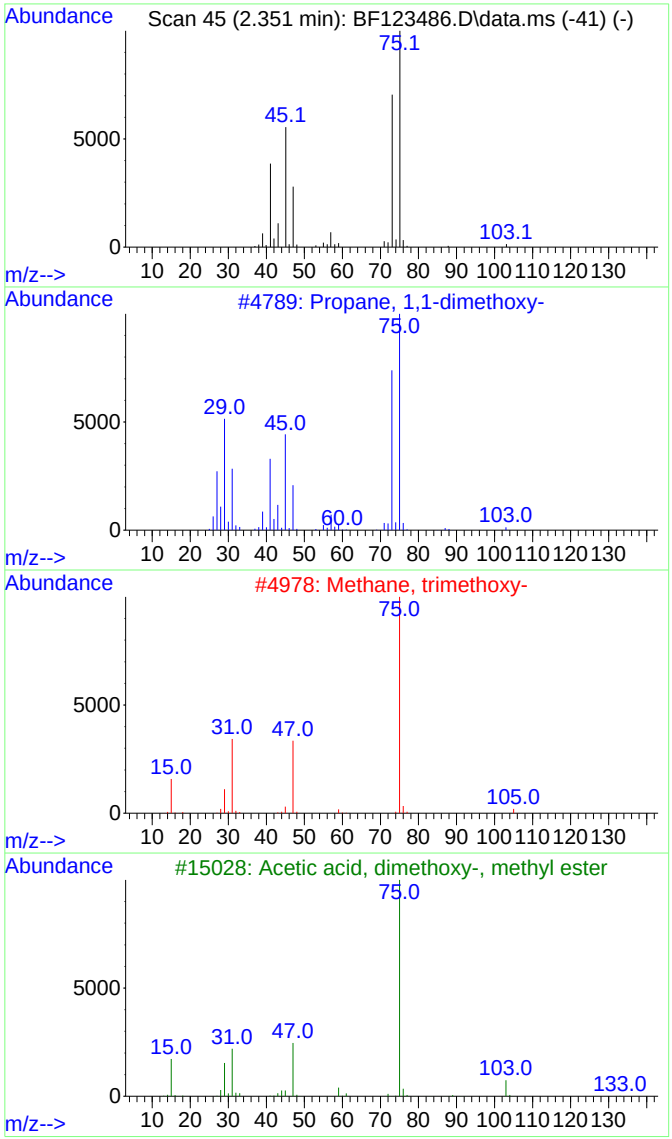
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

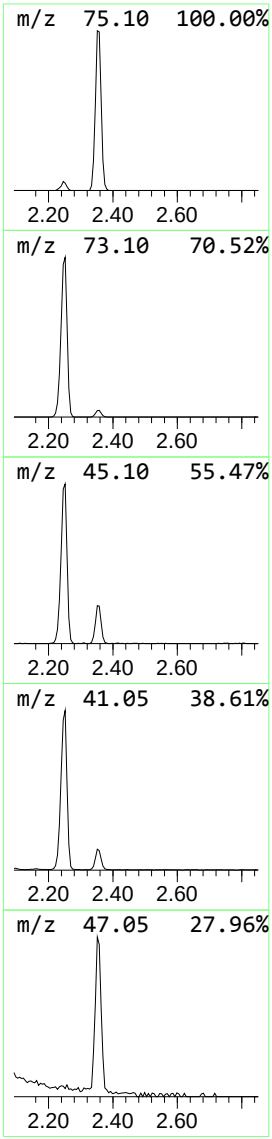
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.351	4.08 ng	294724	1,4-Dichlorobenzene-d4	6.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	Methane, trimethoxy-	106	C4H10O3	000149-73-5	33
3	Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	33
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
5	Boronic acid, ethyl-	74	C2H7BO2	004433-63-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123486.D
Acq On : 26 Mar 2021 15:01
Operator : JU/CG
Sample : M1770-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-104D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

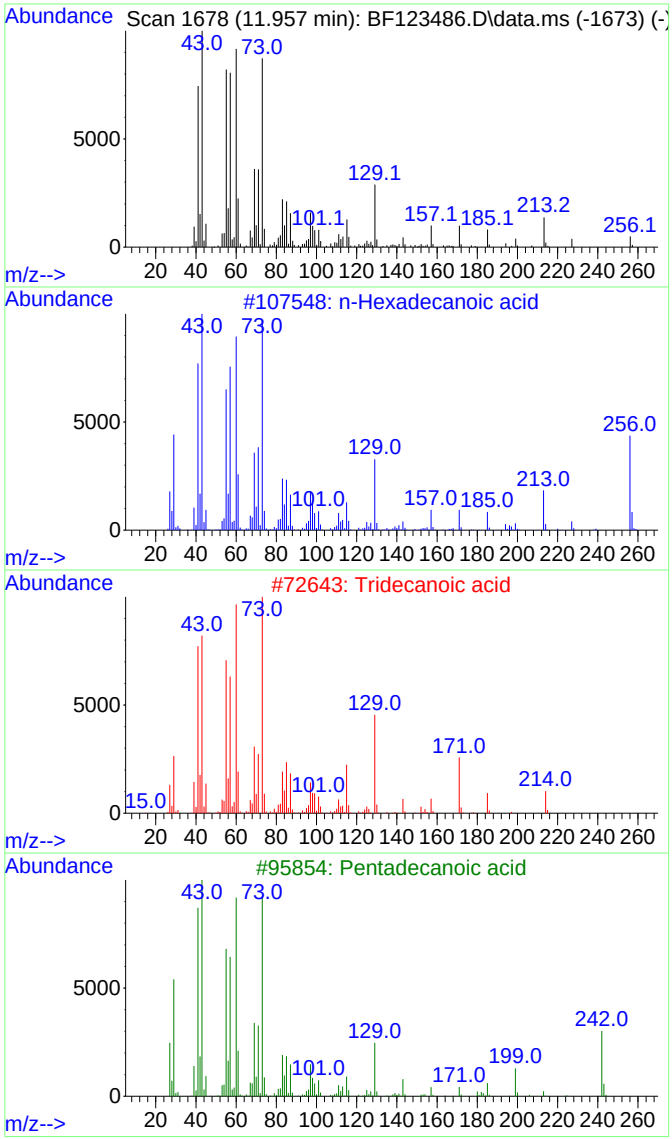
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

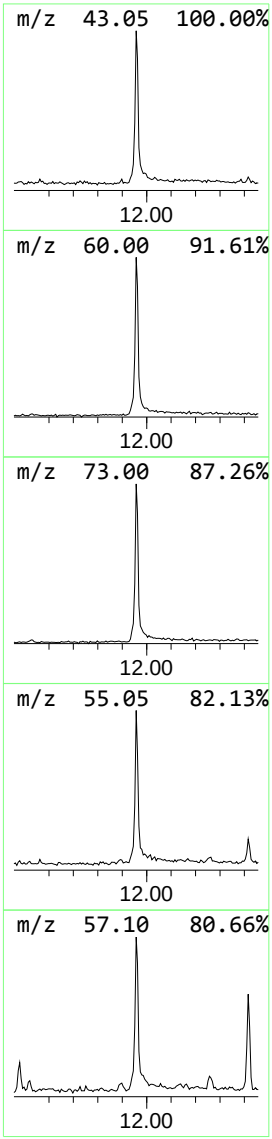
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	6.81 ng	720768	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	78
5	Dodecanoic acid	200	C12H24O2	000143-07-7	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123486.D
Acq On : 26 Mar 2021 15:01
Operator : JU/CG
Sample : M1770-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-104D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

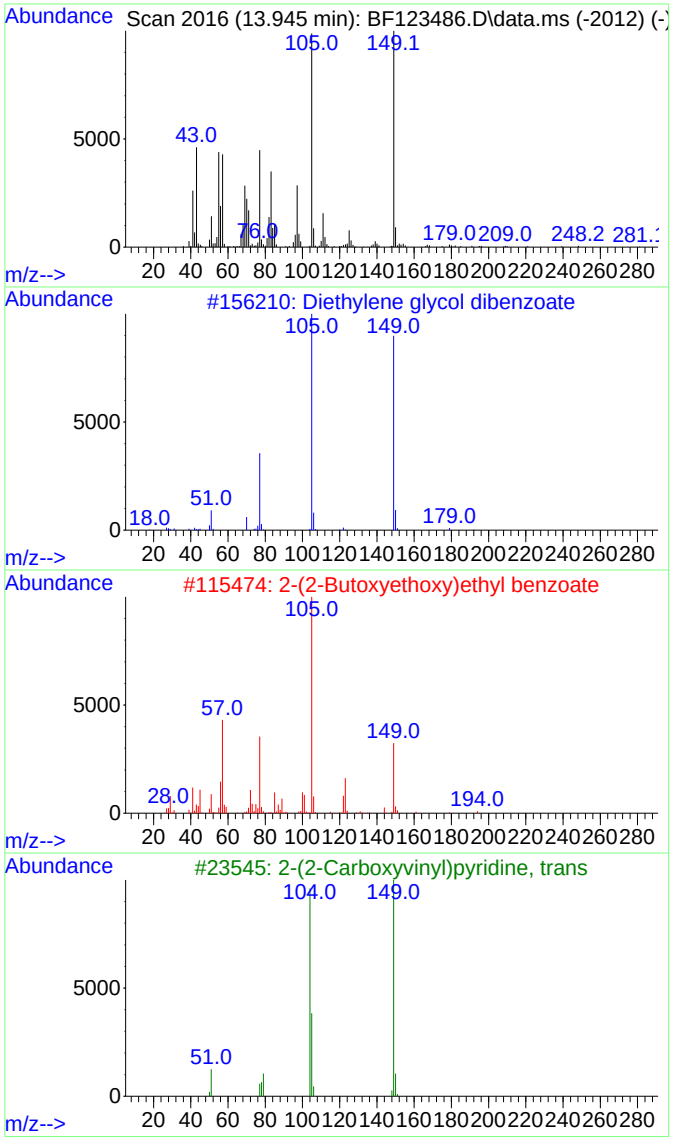
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

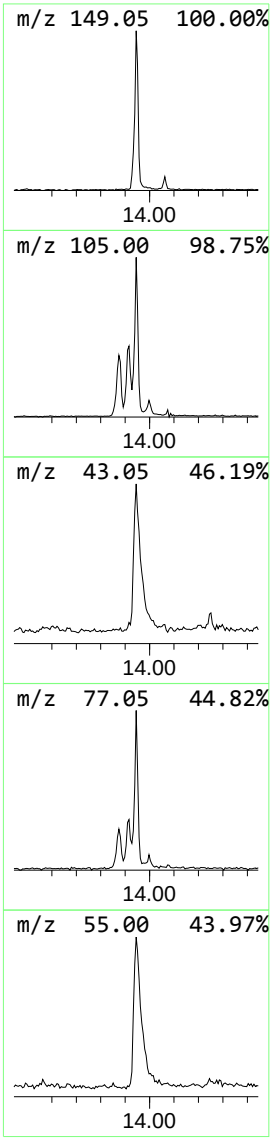
****

Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.945	14.39 ng	1145270	Chrysene-d12	14.080

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	52
2	2-(2-Butoxyethoxy)ethyl benzoate	266	C15H22O4	1000366-98-4	47
3	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	30
4	Vinyl benzoate	148	C9H8O2	000769-78-8	11
5	Ethanone, 1,2-diphenyl-	196	C14H12O	000451-40-1	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
Data File : BF123486.D
Acq On : 26 Mar 2021 15:01
Operator : JU/CG
Sample : M1770-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-104D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.251	62.8	ng	4531850	1	6.898	1444010	20.0
Propane, 1,1-di...	2.351	4.1	ng	294724	1	6.898	1444010	20.0
n-Hexadecanoic ...	11.957	6.8	ng	720768	4	11.433	2116380	20.0
Diethylene glyc...	13.945	14.4	ng	1145270	5	14.080	1591430	20.0