LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136457.D
Acq On : 07 Dec 2023 20:37
Operator : CG\JU
Sample : 05599-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-07

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-BF120523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136457.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	% max.	% of total
1	2.204	17	20	26	rVB	35353	46999	1.81%	0.297%
2	5.040	498	502	508	rVB	49285	62273	2.40%	0.393%
3	5.445	566	571	574	rBV	2518850	2244746	86.59%	14.166%
4	6.445	736	741	744	rBV	2320232	2161886	83.39%	13.644%
5	6.798	798	801	804	rBV	808401	612611	23.63%	3.866%
6	7.363	891	897	899	rBV	1457829	1430902	55.20%	9.030%
7	7.610	937	939	945	rBV	36523	31969	1.23%	0.202%
8	8.075	1014	1018	1021	rBV	997831	764330	29.48%	4.824%
9	8.392	1069	1072	1084	rVB	33407	55604	2.14%	0.351%
10	9.157	1197	1202	1205	rBV	2862645	2592400	100.00%	16.360%
11	9.833	1313	1317	1320	rBV	806513	670584	25.87%	4.232%
12	10.622	1447	1451	1455	rBV	1183371	1052954	40.62%	6.645%
13	11.322	1566	1570	1574	rBV	681256	533985	20.60%	3.370%
14	11.857	1657	1661	1666	rBV2	99368	101427	3.91%	0.640%
15	12.921	1837	1842	1845	rBV	2316522	2027304	78.20%	12.794%
16	13.880	1999	2005	2011	rBV5	45664	112070	4.32%	0.707%
17	13.974	2017	2021	2026	rVB	676536	584088	22.53%	3.686%
18	14.068	2033	2037	2043	rVB2	65738	85680	3.31%	0.541%
19	14.451	2099	2102	2105	rBV3	53019	63526	2.45%	0.401%
20	14.839	2165	2168	2173	rVB3	61462	77323	2.98%	0.488%
21	15.286	2240	2244	2248	rVB3	40229	57971	2.24%	0.366%
22	15.457	2268	2273	2278	rBV	390942	474873	18.32%	2.997%

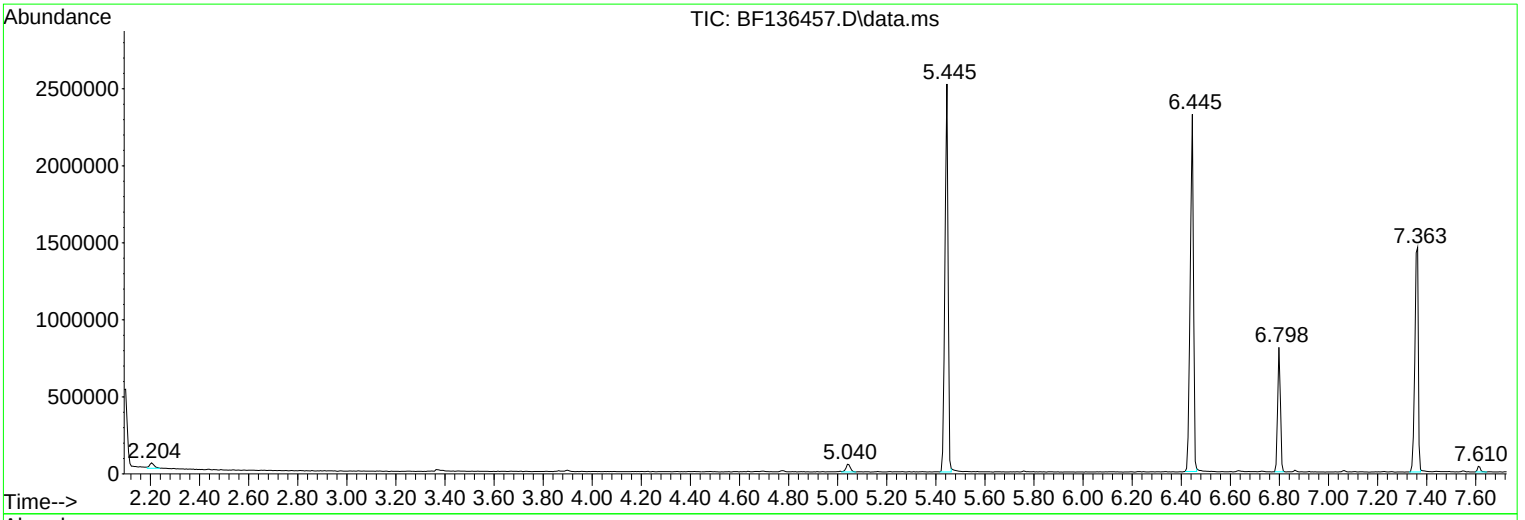
Sum of corrected areas: 15845505

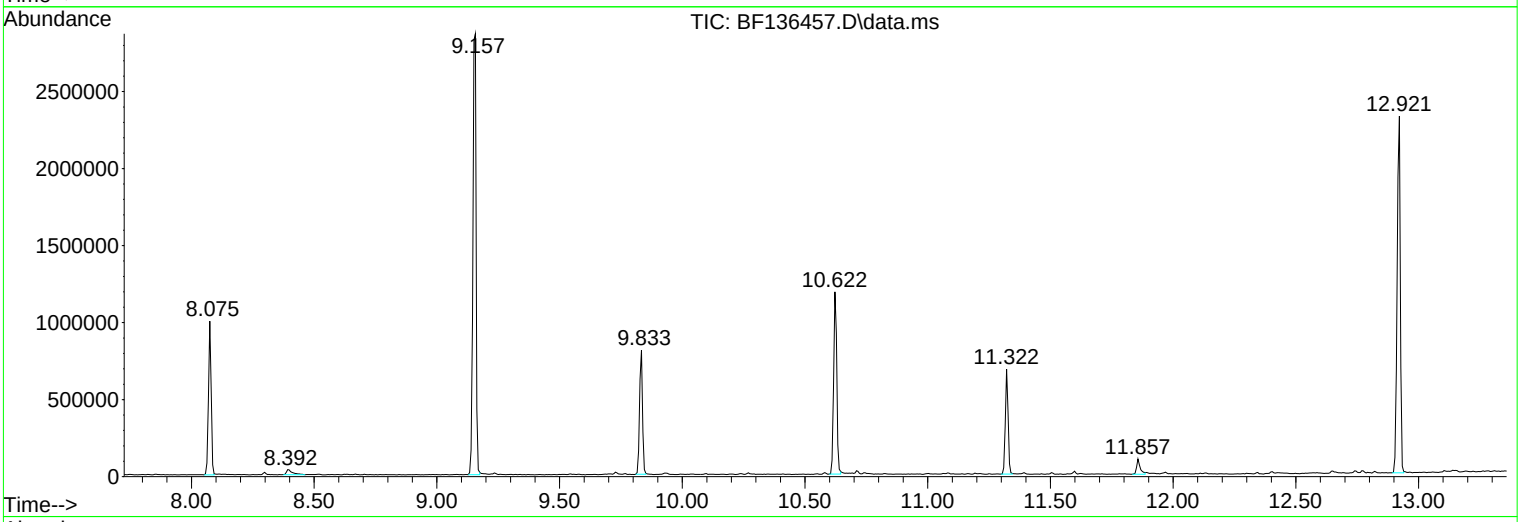
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136457.D
Acq On : 07 Dec 2023 20:37
Operator : CG\JU
Sample : 05599-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

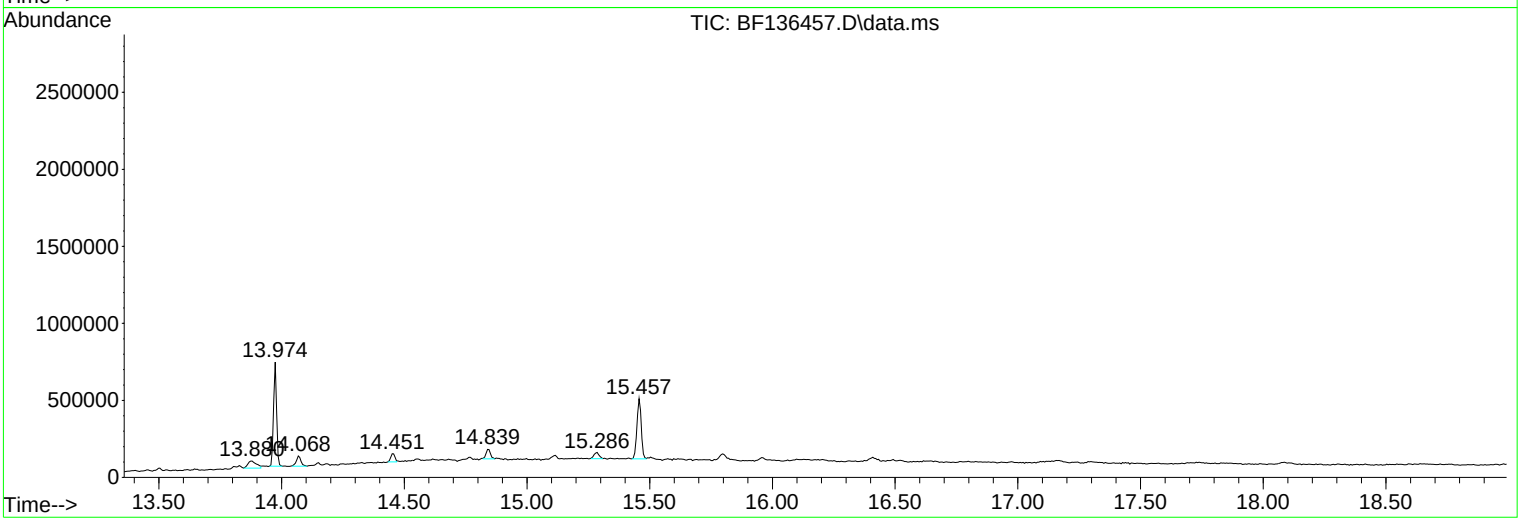
Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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\BF120723\
Data File : BF136457.D
Acq On : 07 Dec 2023 20:37
Operator : CG\JU
Sample : 05599-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-07

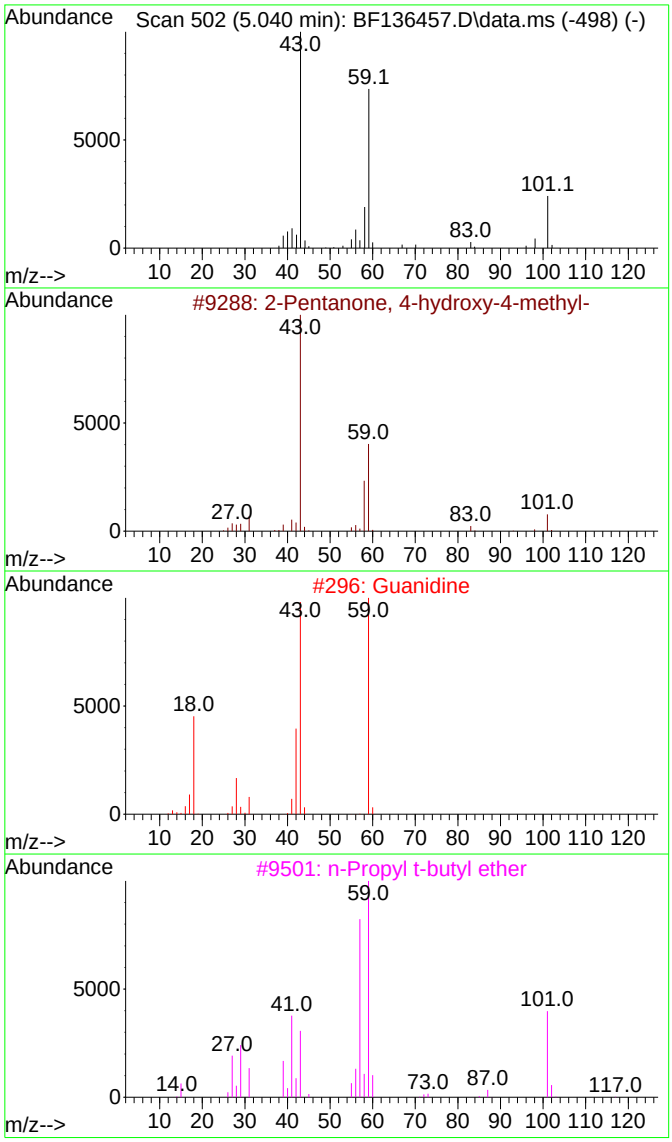
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

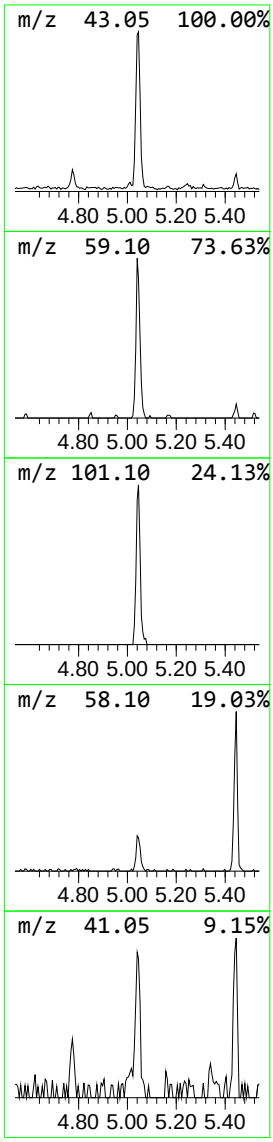
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	2.03 ng	62273	1,4-Dichlorobenzene-d4	6.798

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	47
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136457.D
Acq On : 07 Dec 2023 20:37
Operator : CG\JU
Sample : 05599-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

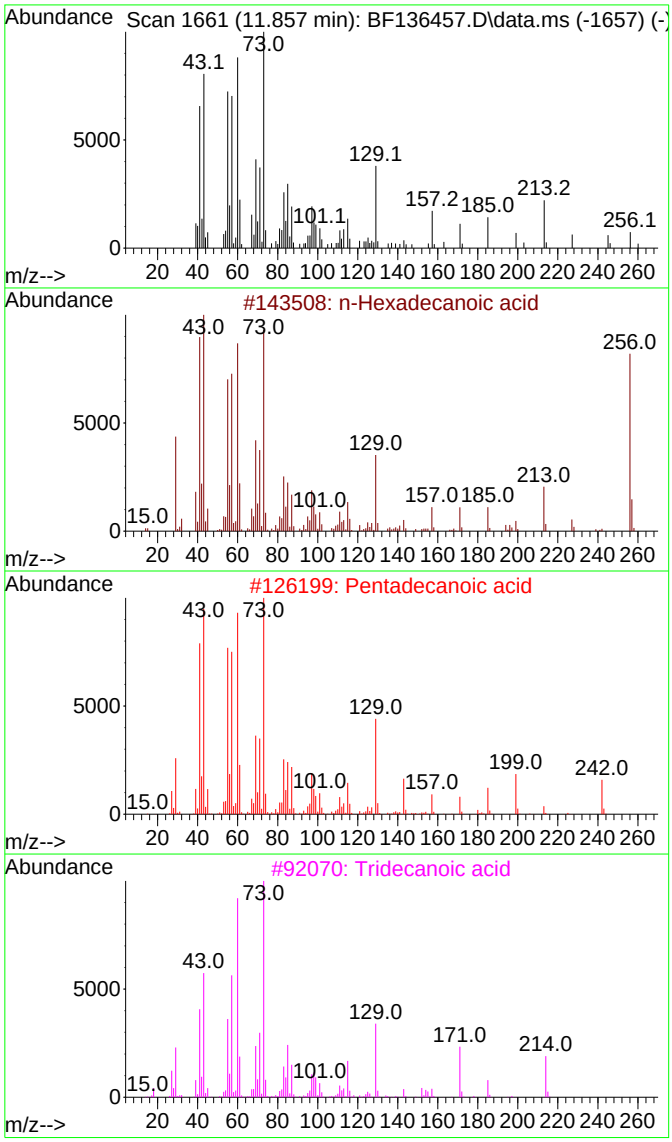
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

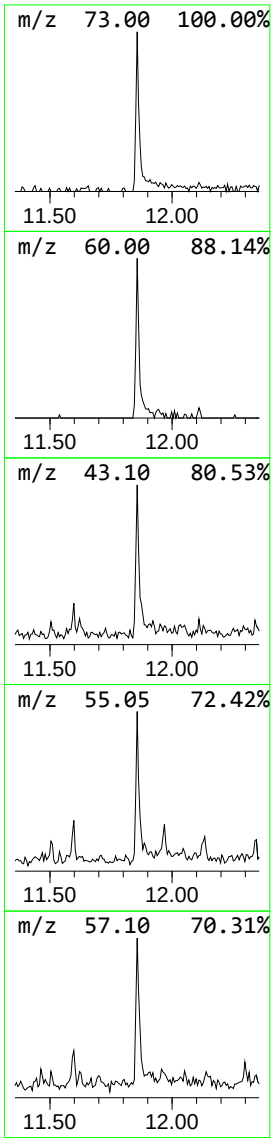
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	3.80 ng	101427	Phenanthrene-d10	11.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
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	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136457.D
Acq On : 07 Dec 2023 20:37
Operator : CG\JU
Sample : 05599-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-07

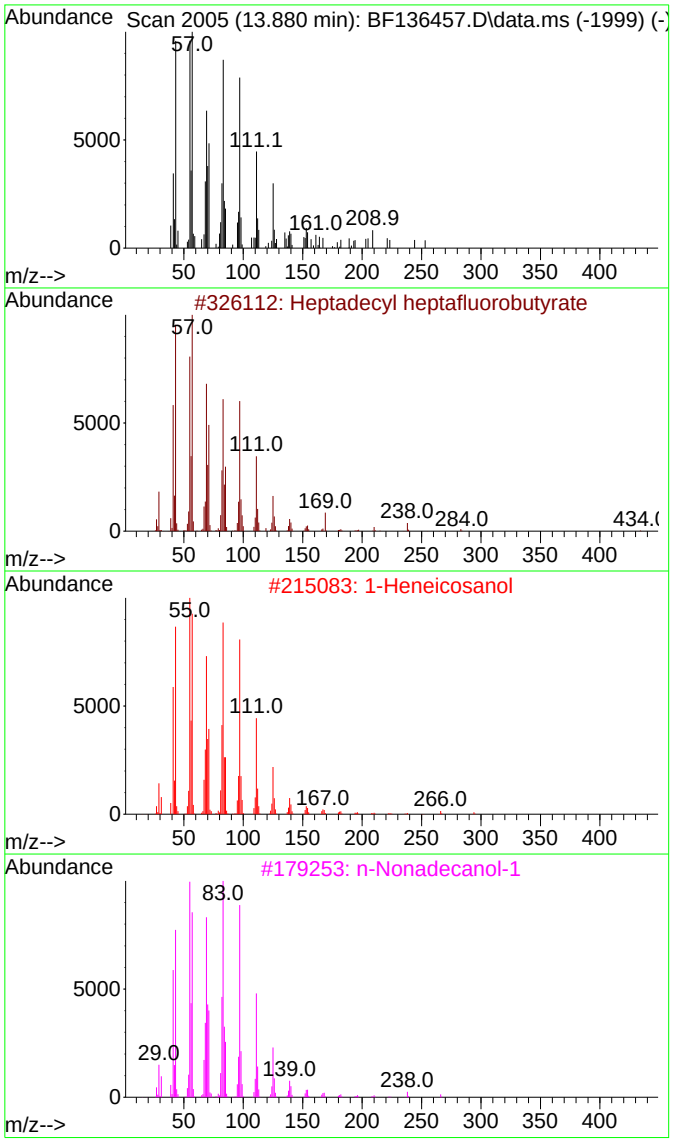
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

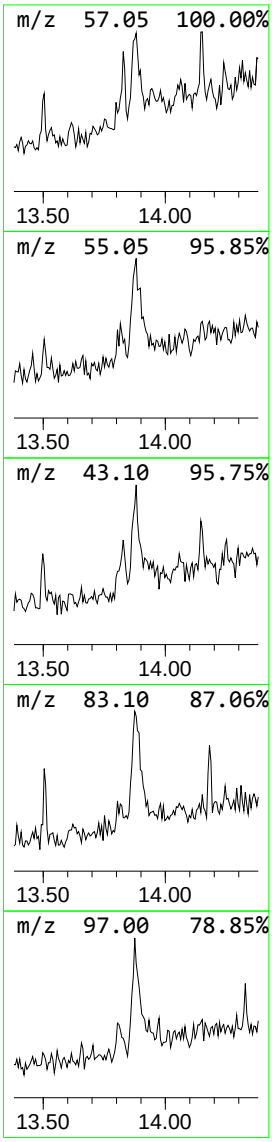
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heptadecyl heptafluorobutyrate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	3.84 ng	112070	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90
2	1-Heneicosanol	312	C21H44O	015594-90-8	87
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	81
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	81
5	1-Tricosene	322	C23H46	018835-32-0	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136457.D
Acq On : 07 Dec 2023 20:37
Operator : CG\JU
Sample : 05599-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

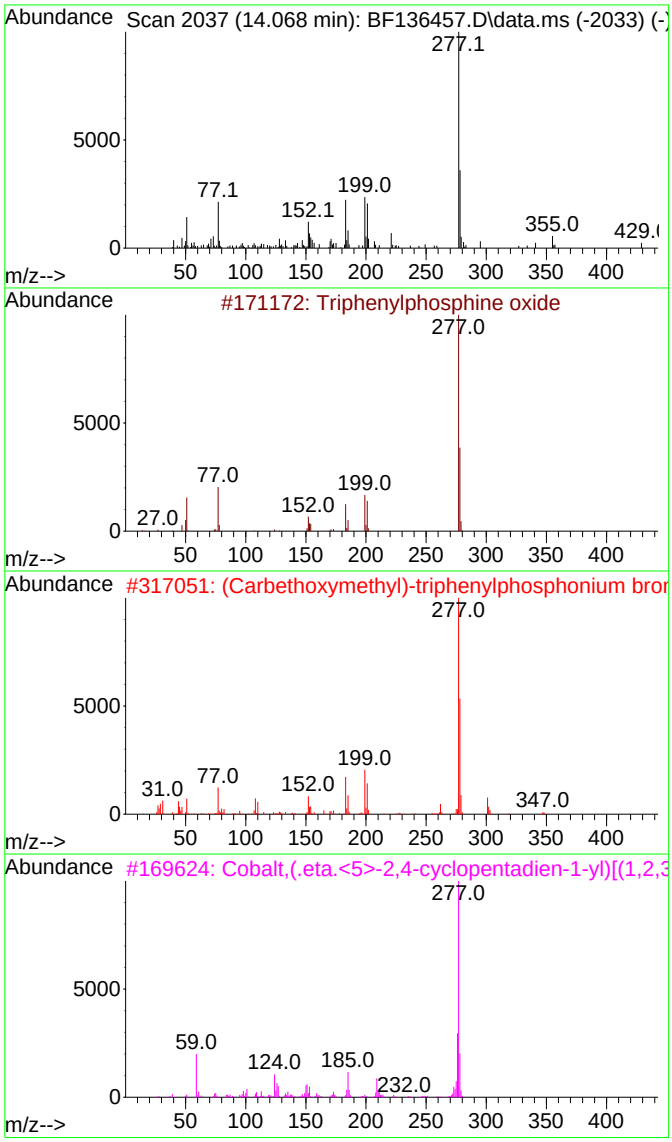
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

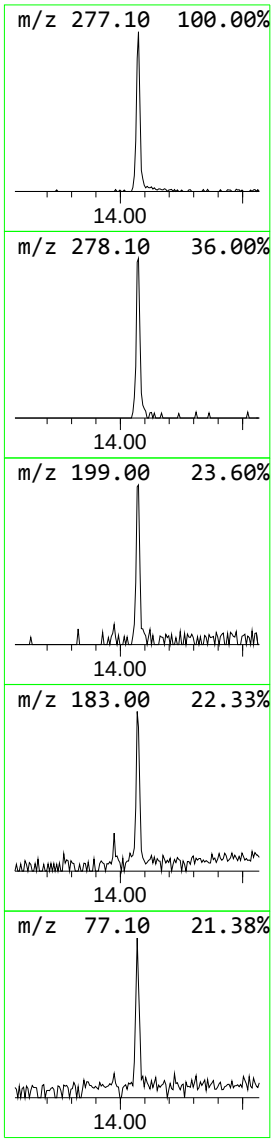
****

Peak Number 4 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.068	2.93 ng	85680	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	45
3	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	43
4	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	43
5	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136457.D
Acq On : 07 Dec 2023 20:37
Operator : CG\JU
Sample : 05599-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

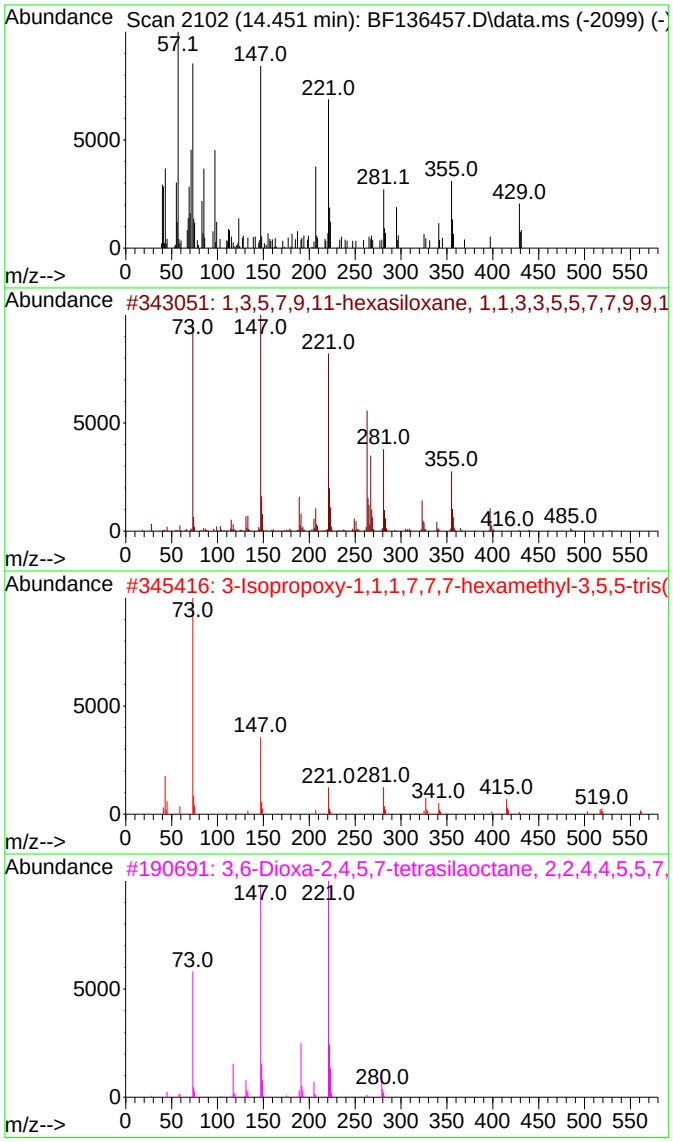
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

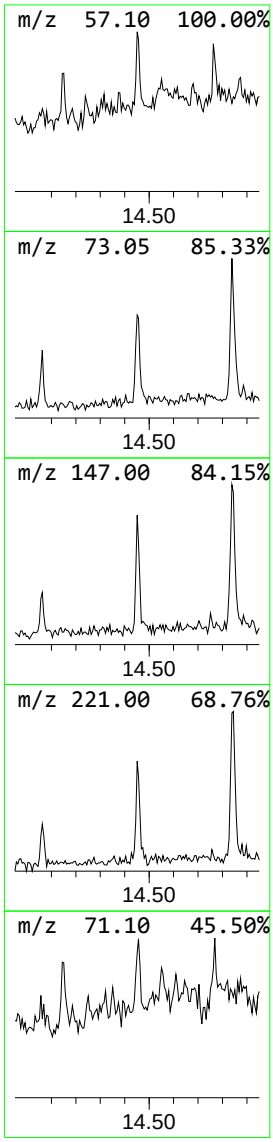
****

Peak Number 5 unknown14.451 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	2.18 ng	63526	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5,7,9,11-hexasiloxane, 1,1,3...	542	C20H54O5Si6	1000458-50-7	40
2	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	32
3	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	25
4	Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	17
5	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136457.D
Acq On : 07 Dec 2023 20:37
Operator : CG\JU
Sample : 05599-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

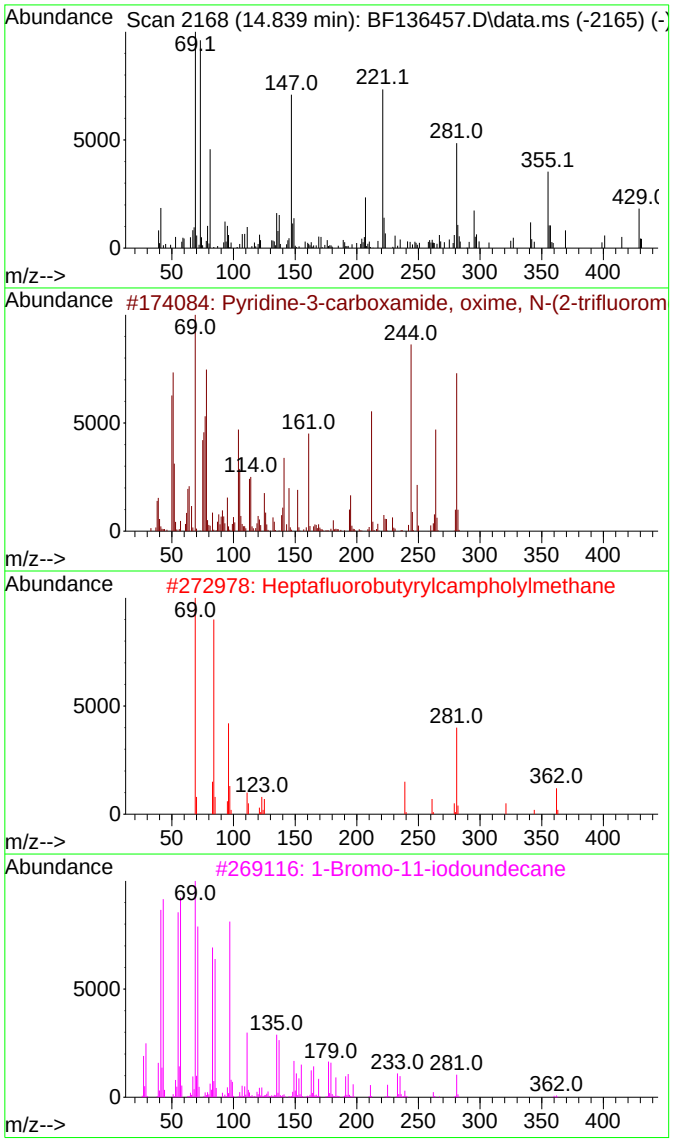
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

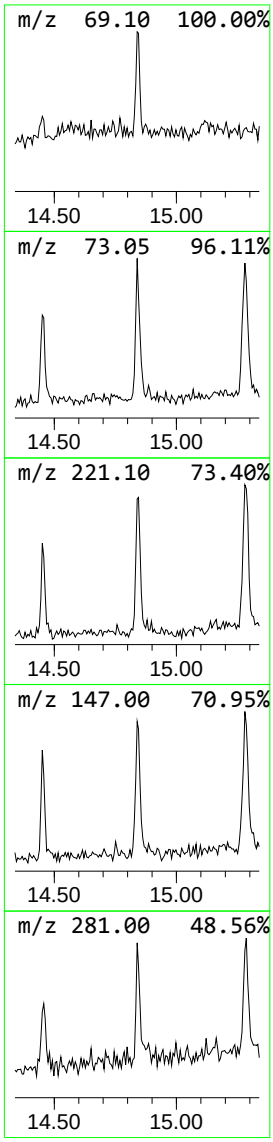
****

Peak Number 6 unknown14.839 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.839	3.26 ng	77323	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine-3-carboxamide, oxime, N...	281	C13H10F3N3O	288246-53-7	27
2	Heptafluorobutyrylcampholylmethane	364	C15H19F7O2	1000098-96-6	27
3	1-Bromo-11-iodoundecane	360	C11H22BrI	139123-69-6	18
4	Ambrox	236	C16H28O	100679-85-4	14
5	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136457.D
Acq On : 07 Dec 2023 20:37
Operator : CG\JU
Sample : 05599-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-07

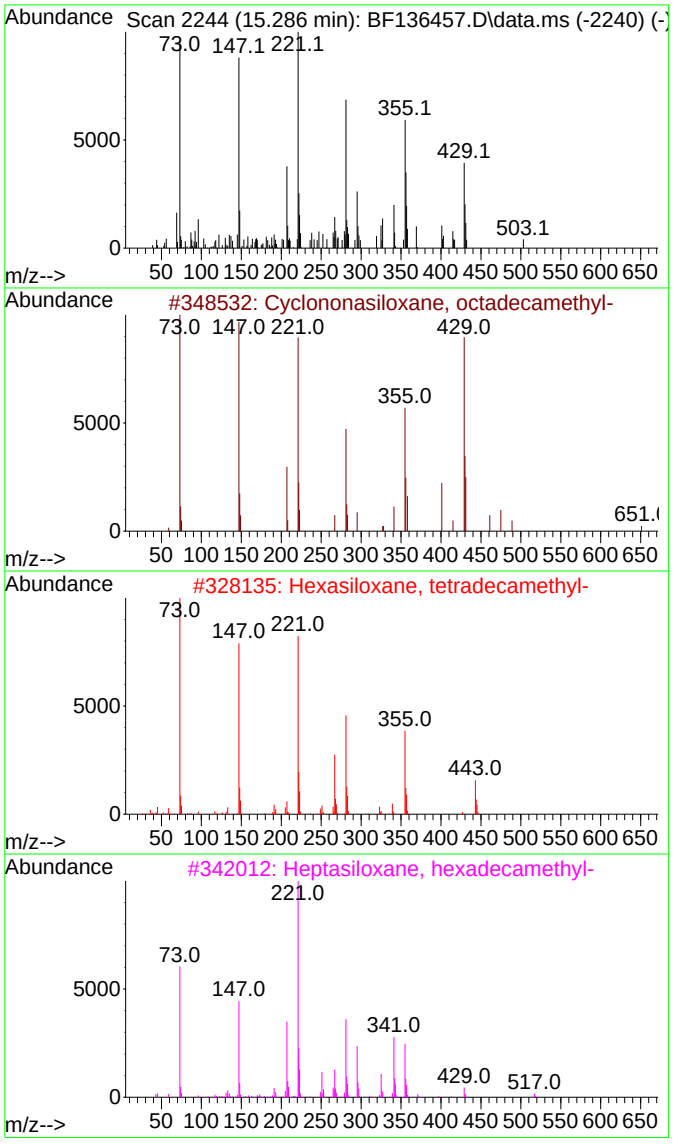
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

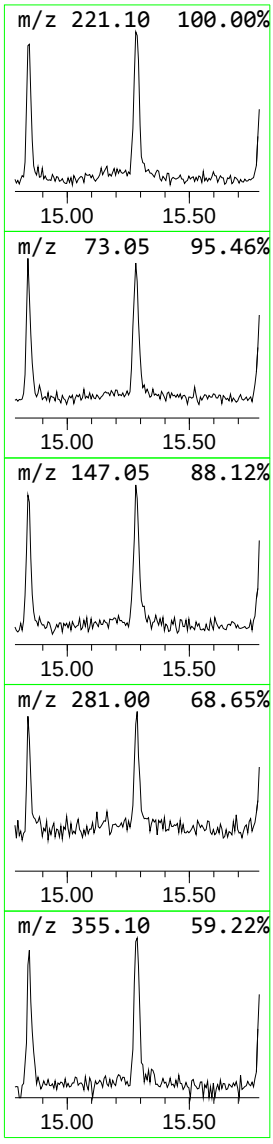
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclononasiloxane, octadeca... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.286	2.44 ng	57971	Perylene-d12	15.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	78
2	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	53
3	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	43
4	1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	40
5	Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136457.D
Acq On : 07 Dec 2023 20:37
Operator : CG\JU
Sample : 05599-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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-...	5.040	2.0	ng	62273	1	6.798	612611	20.0
n-Hexadecanoic ...	11.857	3.8	ng	101427	4	11.322	533985	20.0
Heptadecyl hept...	13.880	3.8	ng	112070	5	13.974	584088	20.0
Triphenylphosph...	14.068	2.9	ng	85680	5	13.974	584088	20.0
unknown14.451	14.451	2.2	ng	63526	5	13.974	584088	20.0
unknown14.839	14.839	3.3	ng	77323	6	15.457	474873	20.0
Cyclononasiloxa...	15.286	2.4	ng	57971	6	15.457	474873	20.0