LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131101.D
Acq On : 09 Nov 2022 22:36
Operator : CG\JU
Sample : N5360-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DISSOLVED-20221175-COMP-10-MODIFIED-ELUTRIATE

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-BF110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131101.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	10	16	22	rVB	1728164	2186777	83.65%	13.858%
2	2.287	30	34	45	rVB3	16606	29757	1.14%	0.189%
3	5.110	510	514	521	rVB	222532	230376	8.81%	1.460%
4	5.510	578	582	585	rBV	1103366	1062749	40.65%	6.735%
5	6.516	748	753	762	rBV	1010378	911493	34.87%	5.776%
6	6.887	813	816	820	rBV	607006	565659	21.64%	3.585%
7	7.457	903	913	916	rBV	1664140	1580819	60.47%	10.018%
8	8.175	1030	1035	1038	rBV	886653	731996	28.00%	4.639%
9	9.251	1212	1218	1221	rBV	2971583	2614107	100.00%	16.566%
10	9.645	1282	1285	1288	rBV	39068	29515	1.13%	0.187%
11	9.934	1328	1334	1337	rBV	1037620	834056	31.91%	5.285%
12	10.728	1464	1469	1472	rBV	1673847	1546969	59.18%	9.803%
13	11.428	1584	1588	1591	rBV	968429	873499	33.41%	5.535%
14	13.010	1853	1857	1860	rBV	1494152	1217376	46.57%	7.715%
15	13.916	2006	2011	2022	rBV	87661	156558	5.99%	0.992%
16	14.069	2033	2037	2041	rBV	737002	627184	23.99%	3.974%
17	14.163	2048	2053	2061	rBV	75345	83014	3.18%	0.526%
18	14.916	2178	2181	2186	rBV2	25471	28773	1.10%	0.182%
19	15.563	2286	2291	2297	rVB	387607	469537	17.96%	2.975%

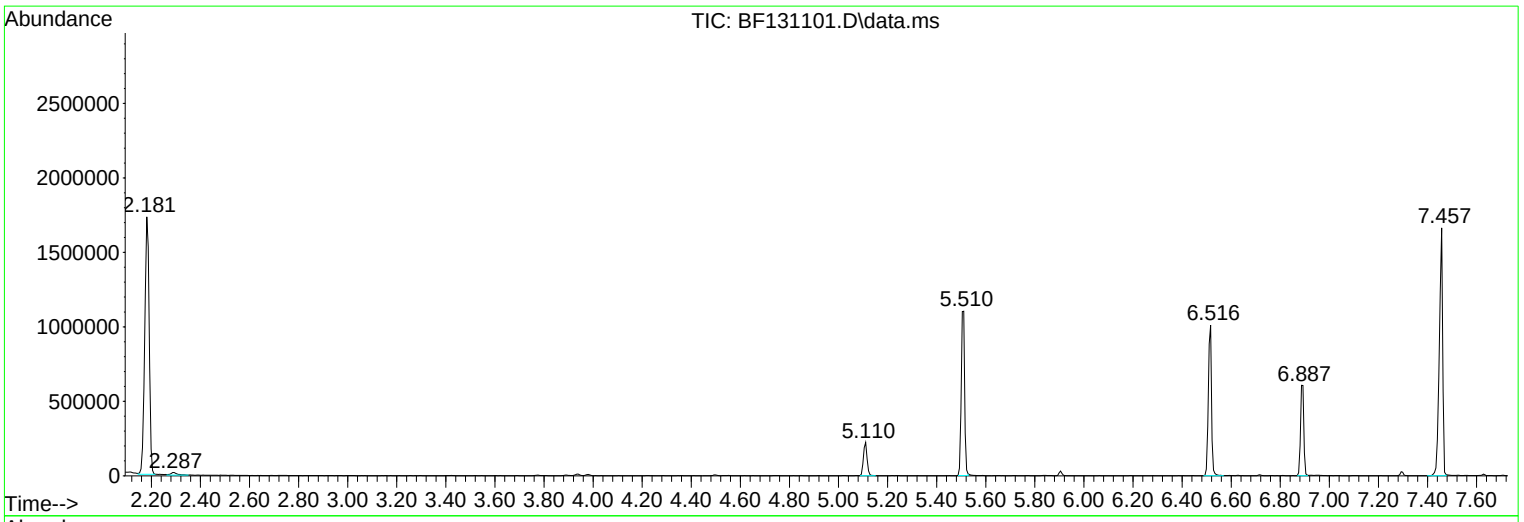
Sum of corrected areas: 15780214

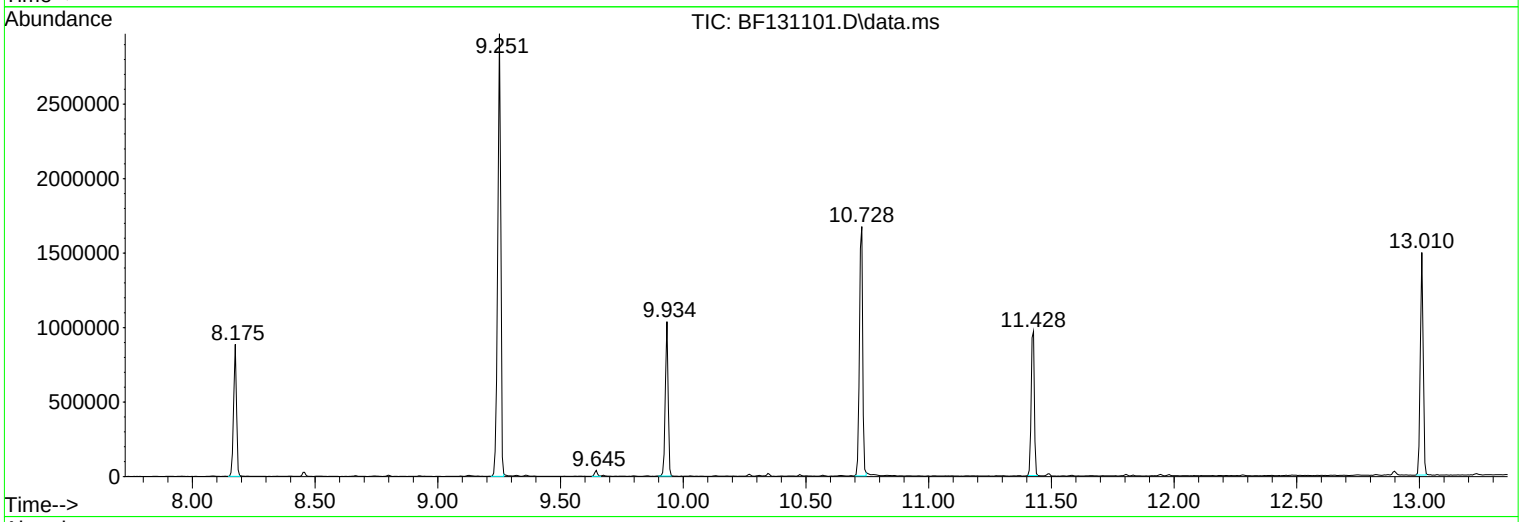
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131101.D
Acq On : 09 Nov 2022 22:36
Operator : CG\JU
Sample : N5360-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

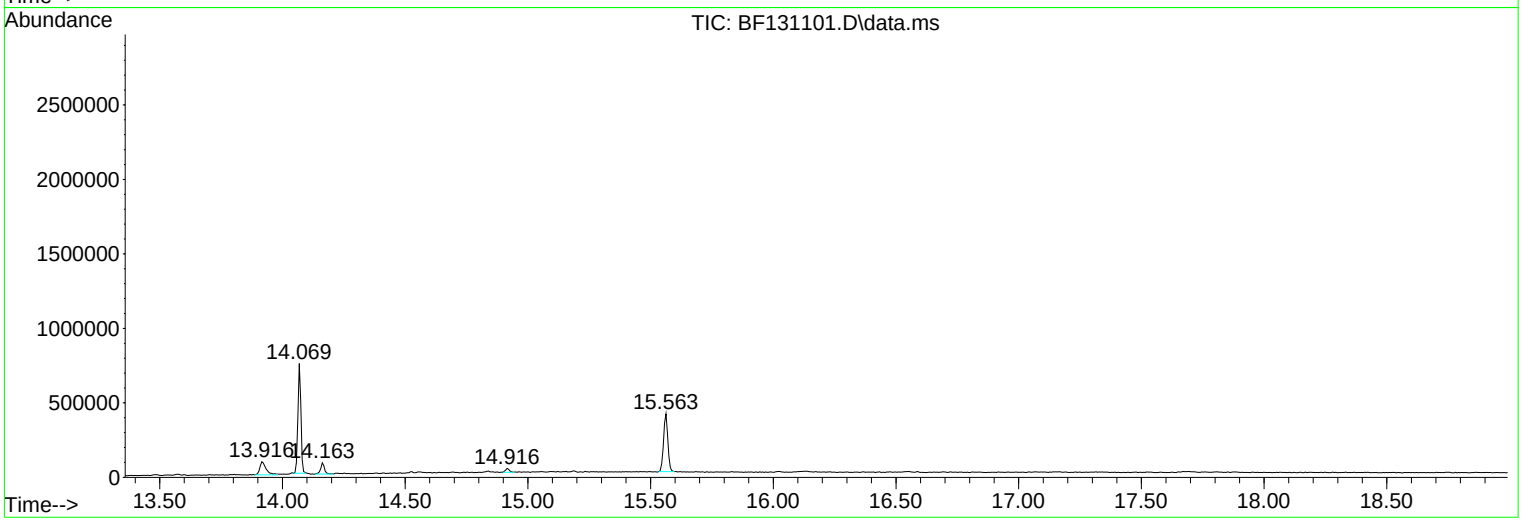
Instrument :
BNA_F
ClientSampleId :
DISSOLVED-20221175-COMP-10-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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\BF110922\
Data File : BF131101.D
Acq On : 09 Nov 2022 22:36
Operator : CG\JU
Sample : N5360-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DISSOLVED-20221175-COMP-10-MODIFIED-ELUTRIATE

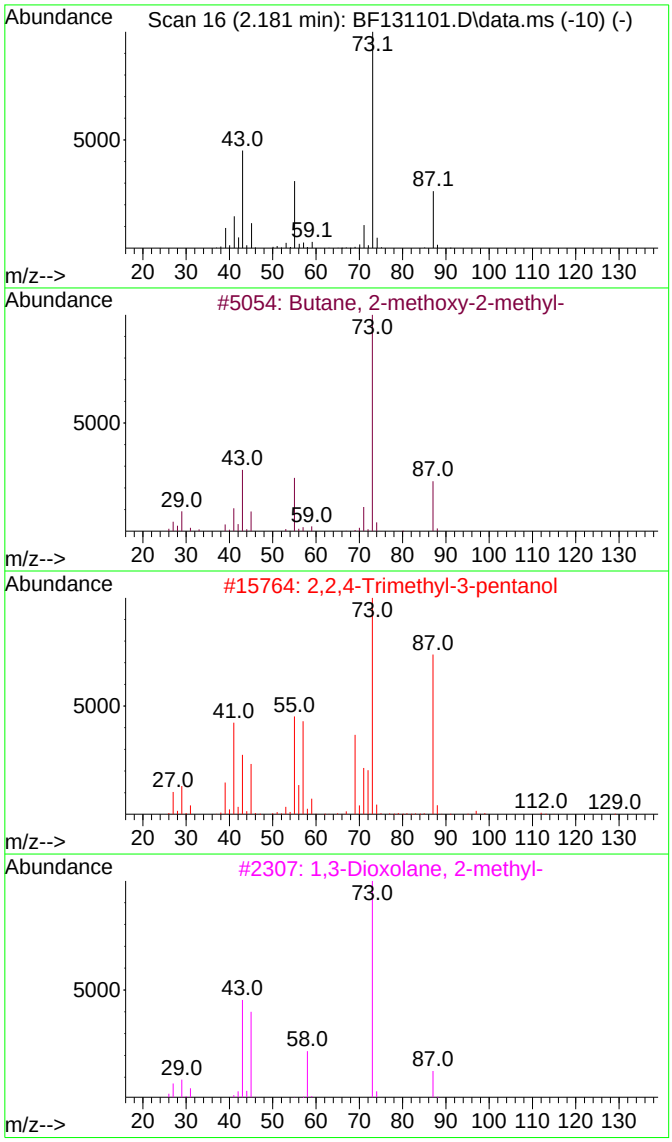
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

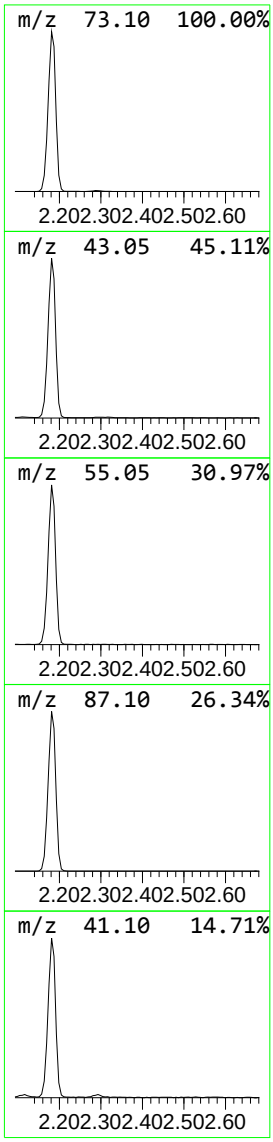
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	77.32 ng	2186780	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131101.D
Acq On : 09 Nov 2022 22:36
Operator : CG\JU
Sample : N5360-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DISSOLVED-20221175-COMP-10-MODIFIED-ELUTRIATE

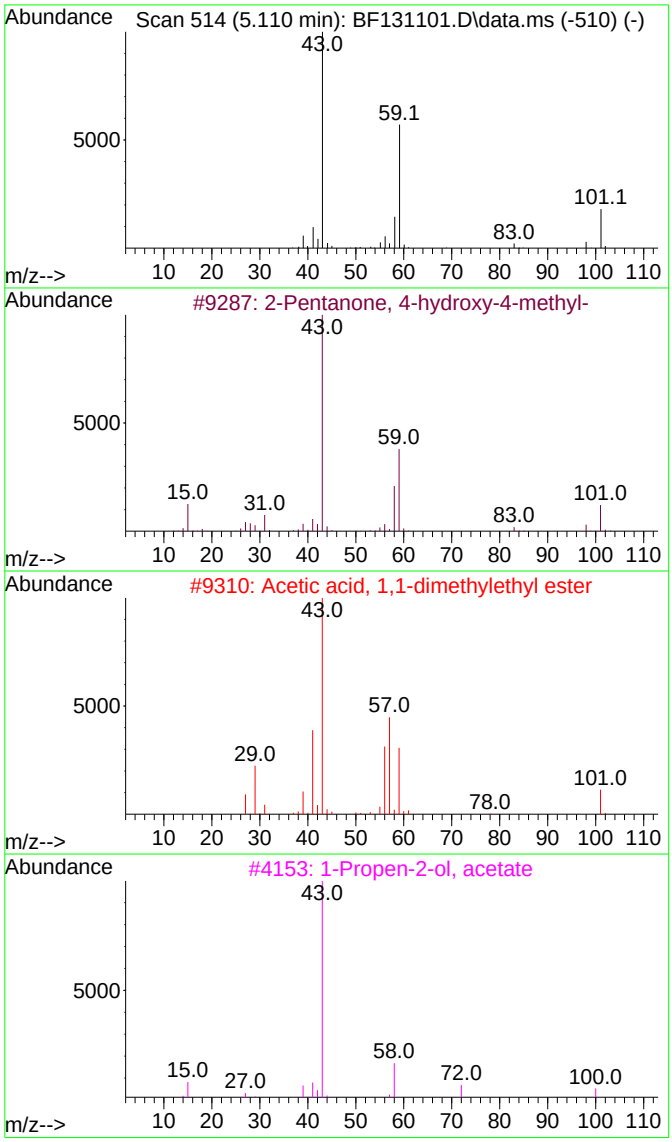
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

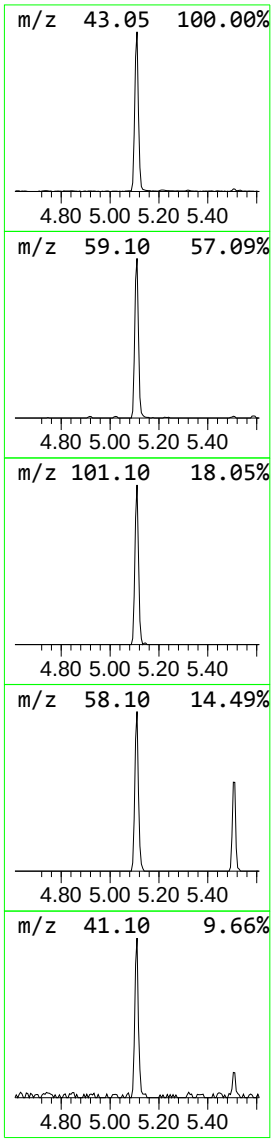
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	8.15 ng	230376	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131101.D
Acq On : 09 Nov 2022 22:36
Operator : CG\JU
Sample : N5360-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DISSOLVED-20221175-COMP-10-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

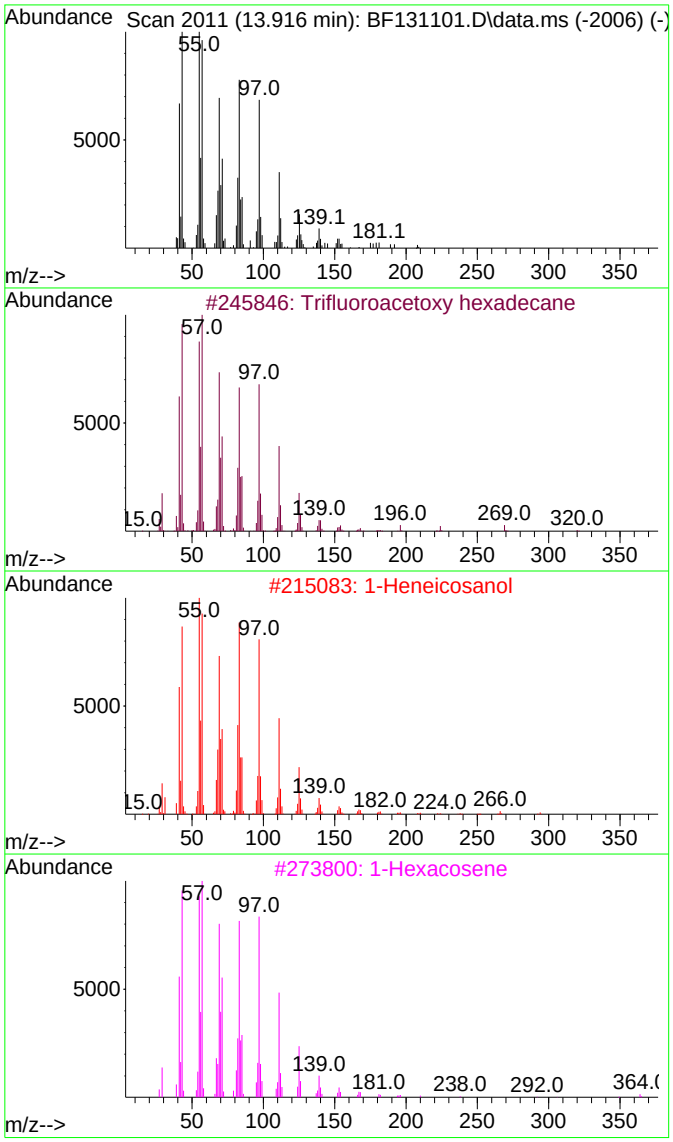
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

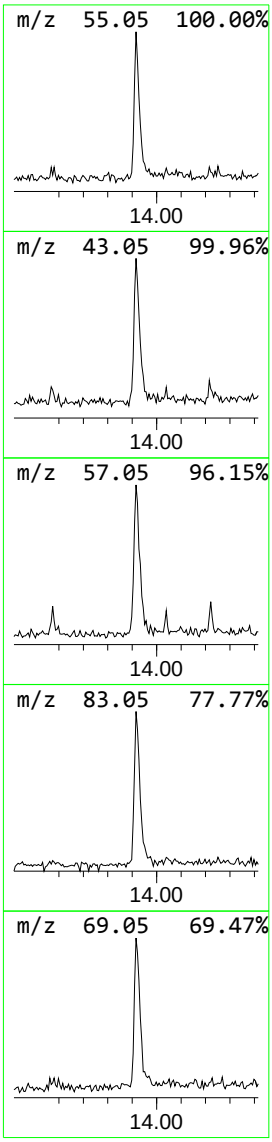
****

Peak Number 3 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	4.99 ng	156558	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	1-Hexacosene	364	C26H52	018835-33-1	93
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	93
5	Octacosanol	410	C28H58O	000557-61-9	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131101.D
Acq On : 09 Nov 2022 22:36
Operator : CG\JU
Sample : N5360-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DISSOLVED-20221175-COMP-10-MODIFIED-ELUTRIATE

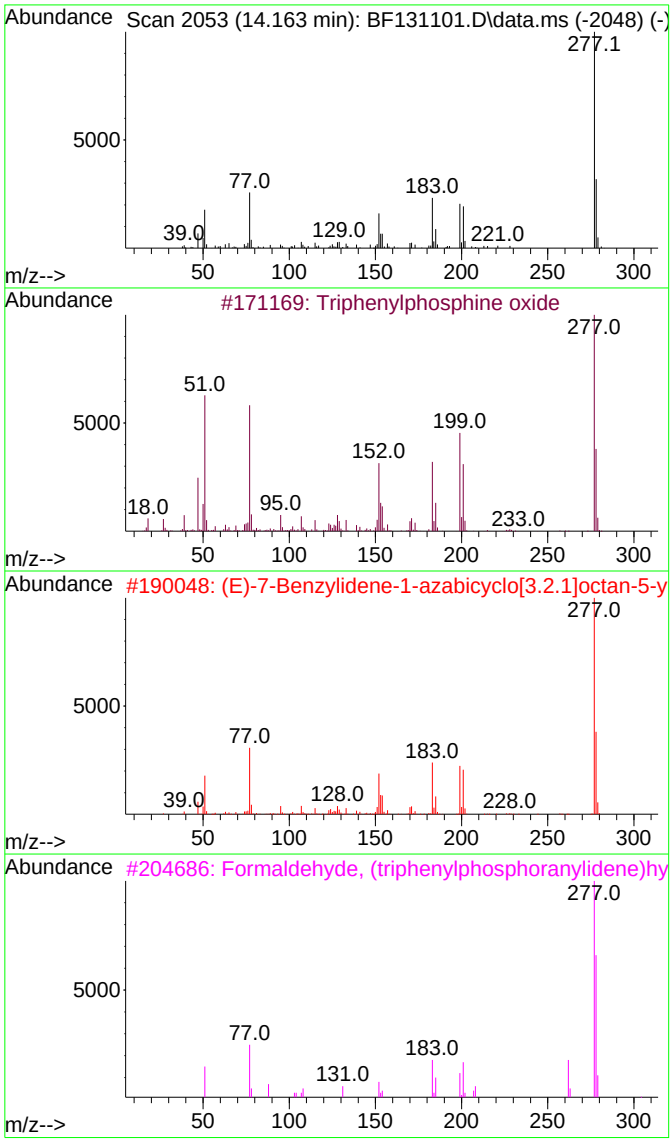
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

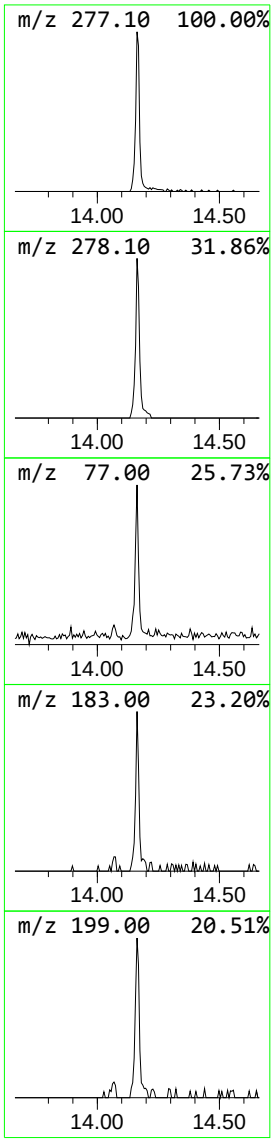
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.163	2.65 ng	83014	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
4	Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38
5	Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110922\
Data File : BF131101.D
Acq On : 09 Nov 2022 22:36
Operator : CG\JU
Sample : N5360-18
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DISSOLVED-20221175-COMP-10-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110922.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...	2.181	77.3	ng	2186780	1	6.893	565659	20.0
2-Pentanone, 4-...	5.110	8.2	ng	230376	1	6.893	565659	20.0
Trifluoroacetox...	13.916	5.0	ng	156558	5	14.069	627184	20.0
Triphenylphosph...	14.163	2.6	ng	83014	5	14.069	627184	20.0