LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131968.D
Acq On : 09 Jan 2023 17:52
Operator : CG\JU
Sample : 01043-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-203

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-BF010923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131968.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	6	10	17	rVB	57164	83225	2.79%	0.415%
2	4.998	488	495	504	rVB	707149	1032196	34.59%	5.151%
3	5.404	559	564	567	rBV	2395972	2339766	78.42%	11.677%
4	6.428	732	738	741	rBV	2299225	2386170	79.97%	11.908%
5	6.781	795	798	802	rBV	557073	494506	16.57%	2.468%
6	7.357	890	896	899	rBV	1564216	1600221	53.63%	7.986%
7	8.075	1013	1018	1021	rBV	700553	631041	21.15%	3.149%
8	9.157	1196	1202	1205	rBV	3310023	2983713	100.00%	14.890%
9	9.833	1309	1317	1320	rBV	926048	777284	26.05%	3.879%
10	9.969	1337	1340	1345	rBV	162375	140724	4.72%	0.702%
11	10.551	1434	1439	1443	rBV	99215	88776	2.98%	0.443%
12	10.627	1446	1452	1456	rBV	2011085	2071974	69.44%	10.340%
13	10.974	1507	1511	1518	rVB7	23124	36282	1.22%	0.181%
14	11.327	1567	1571	1574	rVB	908279	809001	27.11%	4.037%
15	11.857	1654	1661	1664	rBV	127478	160856	5.39%	0.803%
16	12.004	1682	1686	1688	rBV	51125	62567	2.10%	0.312%
17	12.033	1688	1691	1700	rVB2	75146	110883	3.72%	0.553%
18	12.104	1700	1703	1711	rVB	60629	54175	1.82%	0.270%
19	12.921	1837	1842	1845	rBV	3420133	2964337	99.35%	14.794%
20	13.486	1931	1938	1941	rVB2	24483	35023	1.17%	0.175%
21	13.815	1990	1994	2009	rBV	182264	247535	8.30%	1.235%
22	13.974	2017	2021	2025	rVB	588014	492570	16.51%	2.458%
23	14.745	2147	2152	2156	rVB5	19988	36319	1.22%	0.181%
24	15.439	2265	2270	2276	rVB	325818	398938	13.37%	1.991%

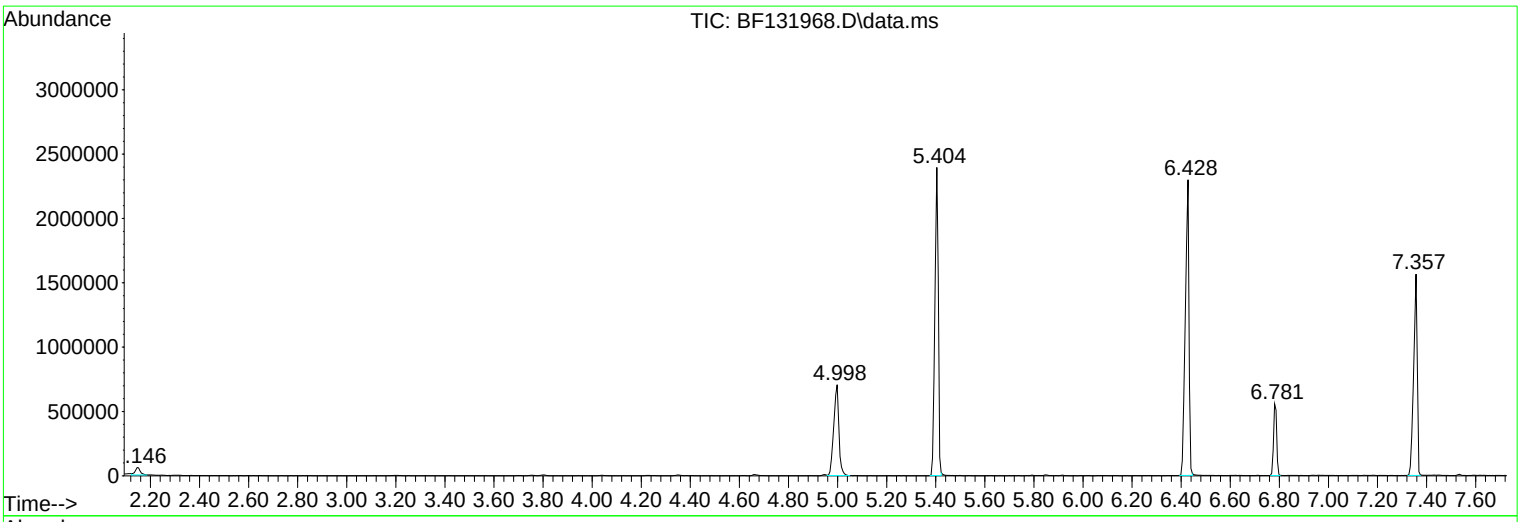
Sum of corrected areas: 20038082

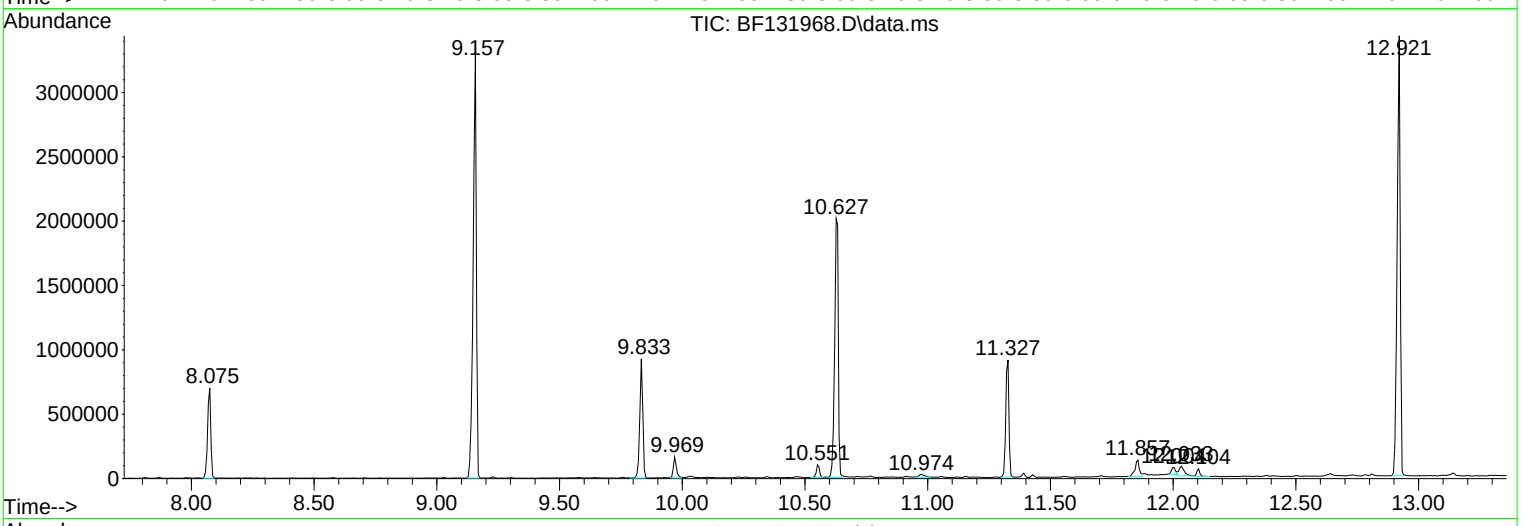
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131968.D
Acq On : 09 Jan 2023 17:52
Operator : CG\JU
Sample : 01043-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

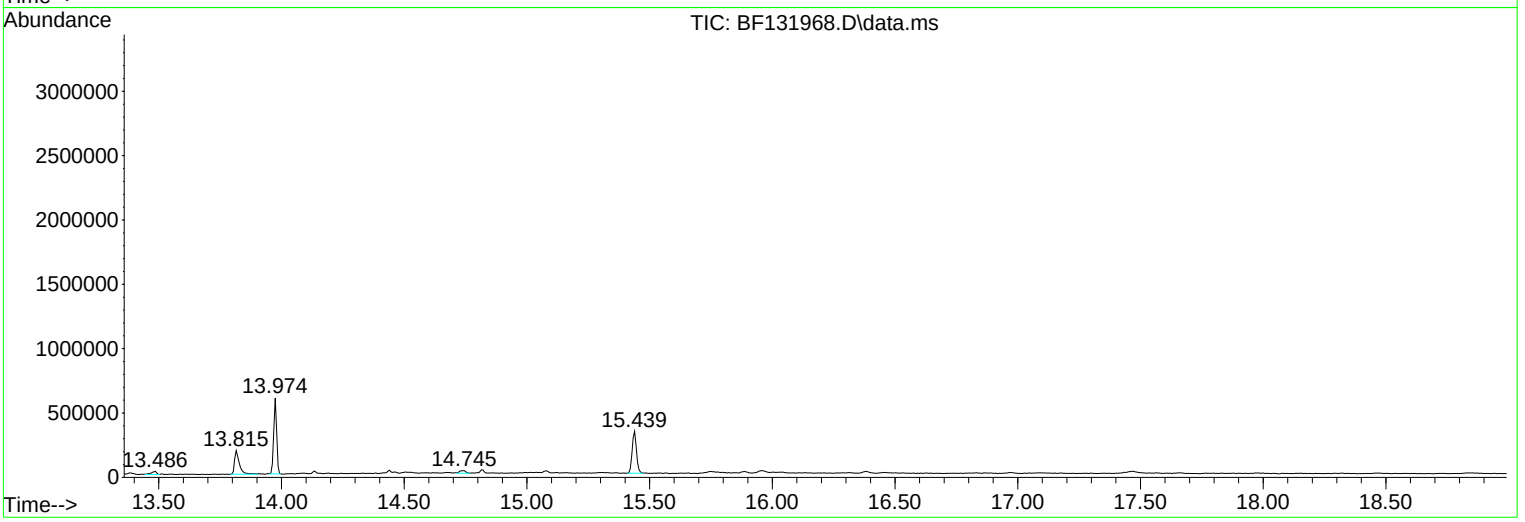
Instrument :
BNA_F
ClientSampleId :
TP-203

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.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\BF010923\
Data File : BF131968.D
Acq On : 09 Jan 2023 17:52
Operator : CG\JU
Sample : 01043-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-203

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

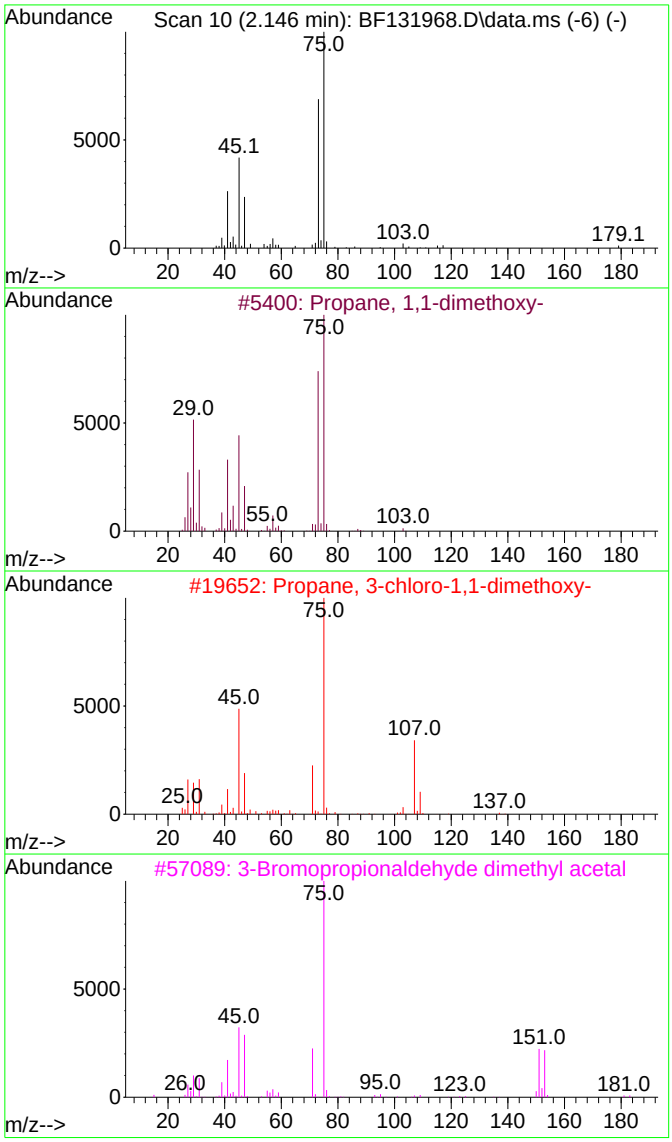
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

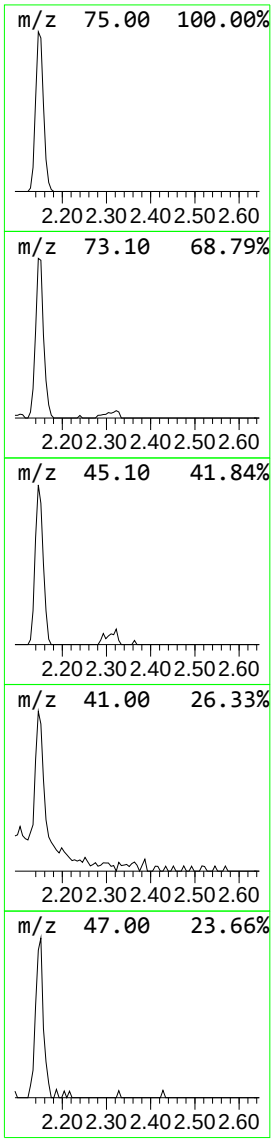
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	3.37 ng	83225	1,4-Dichlorobenzene-d4	6.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2	Propane, 3-chloro-1,1-dimethoxy-	138	C5H11ClO2	035502-06-8	40
3	3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	38
4	Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	36
5	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131968.D
Acq On : 09 Jan 2023 17:52
Operator : CG\JU
Sample : 01043-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-203

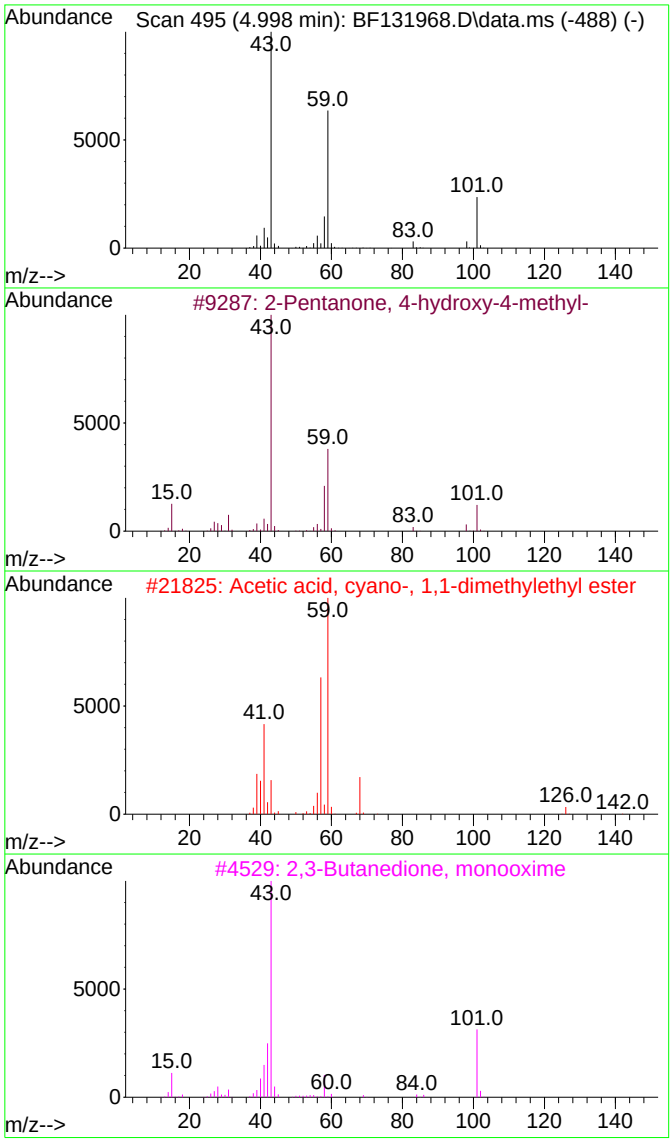
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

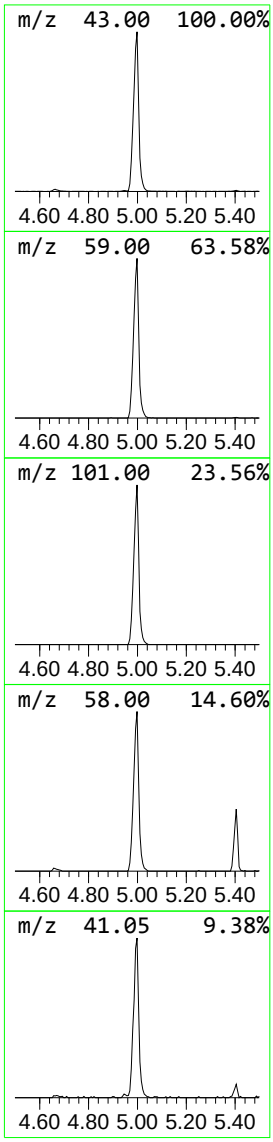
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.998	41.75 ng	1032200	1,4-Dichlorobenzene-d4	6.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
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\BF010923\
Data File : BF131968.D
Acq On : 09 Jan 2023 17:52
Operator : CG\JU
Sample : 01043-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-203

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

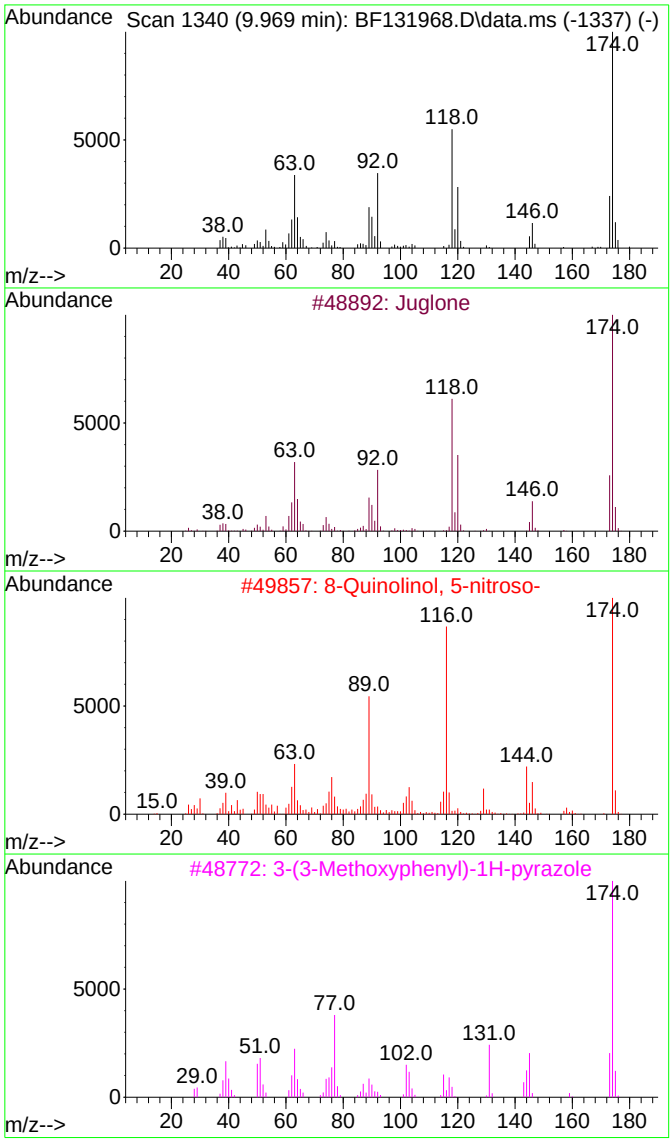
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

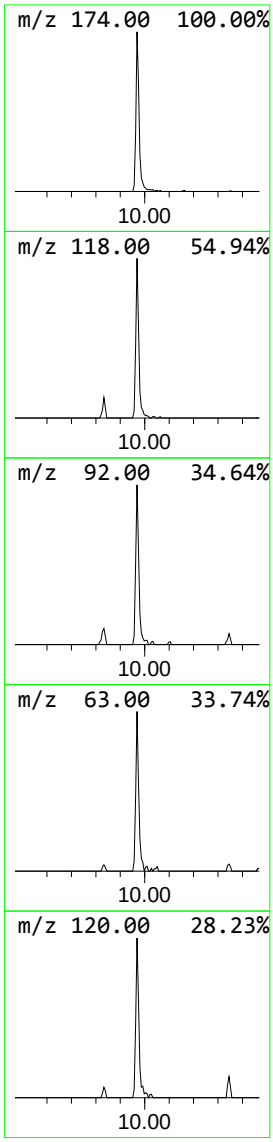
****

Peak Number 3 Juglone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.969	3.62 ng	140724	Acenaphthene-d10	9.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Juglone	174	C10H6O3	000481-39-0	98
2	8-Quinolinol, 5-nitroso-	174	C9H6N2O2	003565-26-2	43
3	3-(3-Methoxyphenyl)-1H-pyrazole	174	C10H10N2O	1000410-63-5	43
4	Benzene, 2,4-diisocyanato-1-methyl-	174	C9H6N2O2	000584-84-9	38
5	1-(3-Pyridinylmethyl)-3-piperidi...	275	C16H25N3O	1000469-14-7	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131968.D
Acq On : 09 Jan 2023 17:52
Operator : CG\JU
Sample : 01043-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-203

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

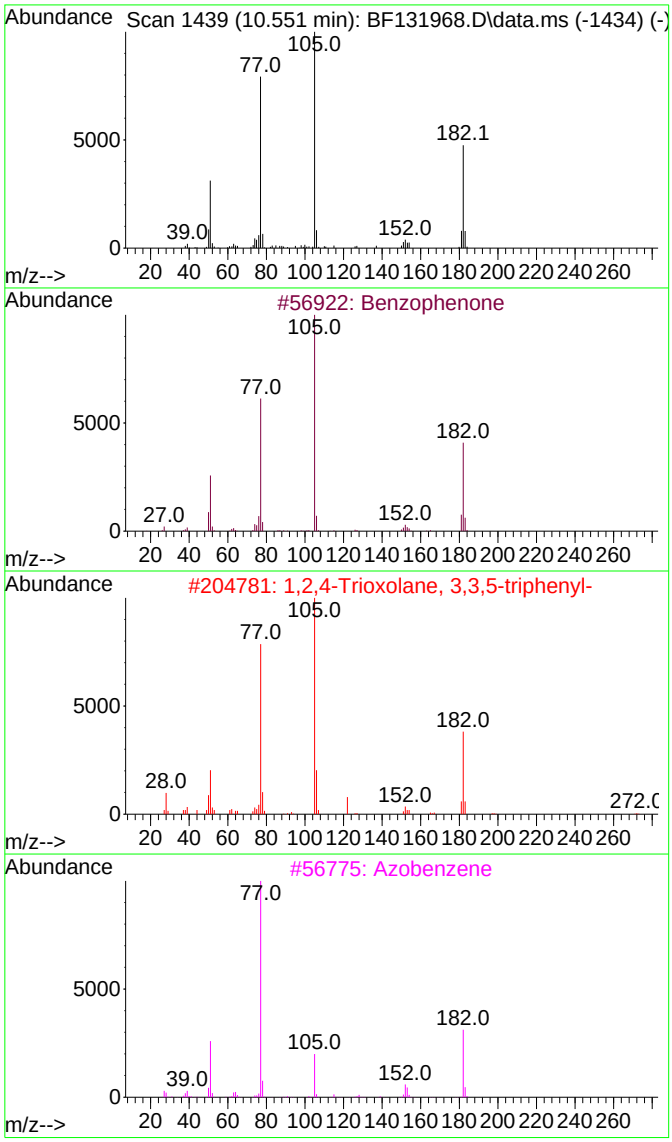
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

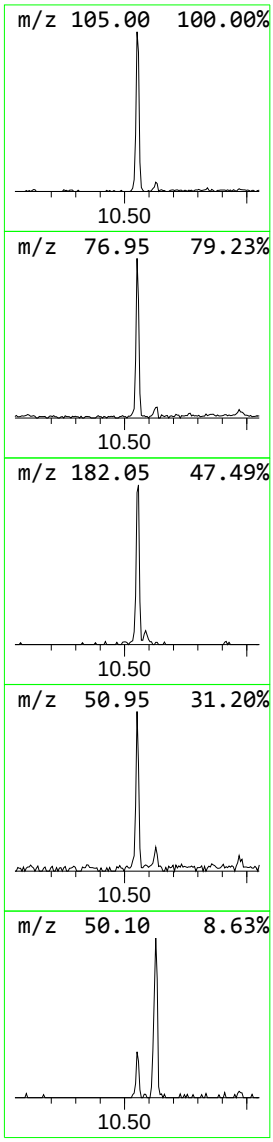
****

Peak Number 4 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.551	2.28 ng	88776	Acenaphthene-d10	9.833

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	83
3	Azobenzene	182	C12H10N2	000103-33-3	64
4	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	53
5	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131968.D
Acq On : 09 Jan 2023 17:52
Operator : CG\JU
Sample : 01043-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-203

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

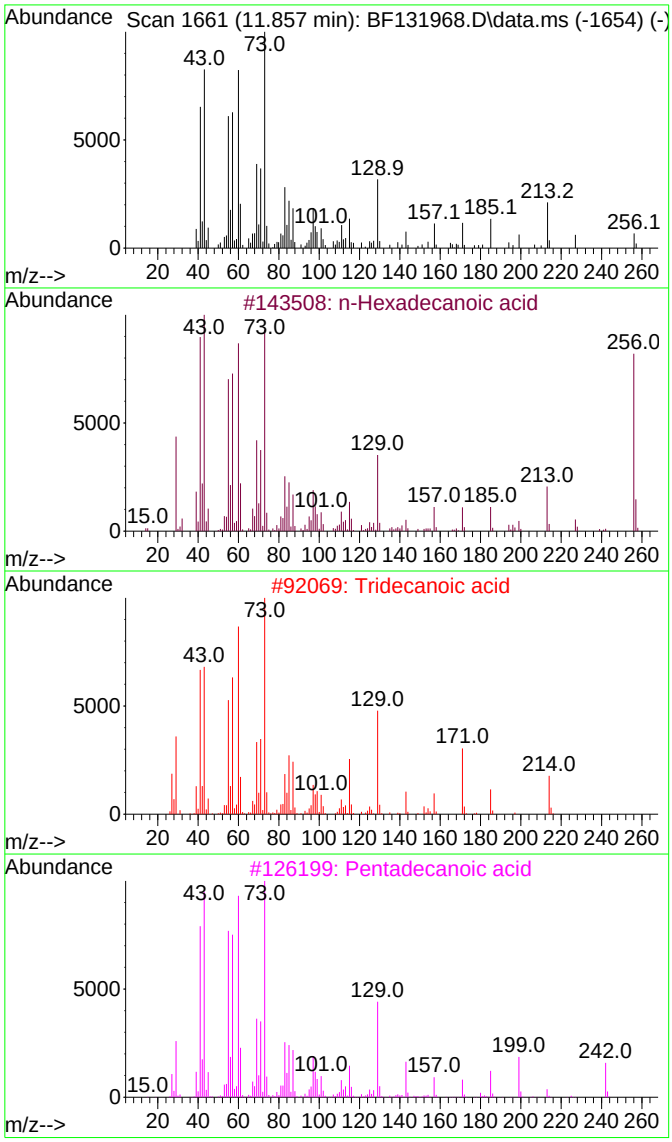
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

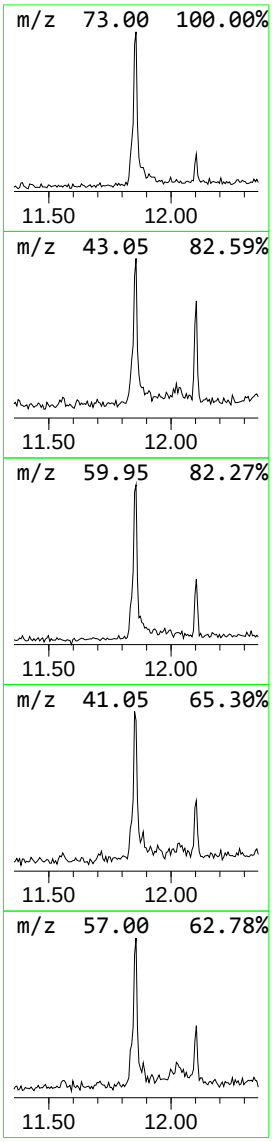
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	3.98 ng	160856	Phenanthrene-d10	11.327

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131968.D
Acq On : 09 Jan 2023 17:52
Operator : CG\JU
Sample : 01043-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-203

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

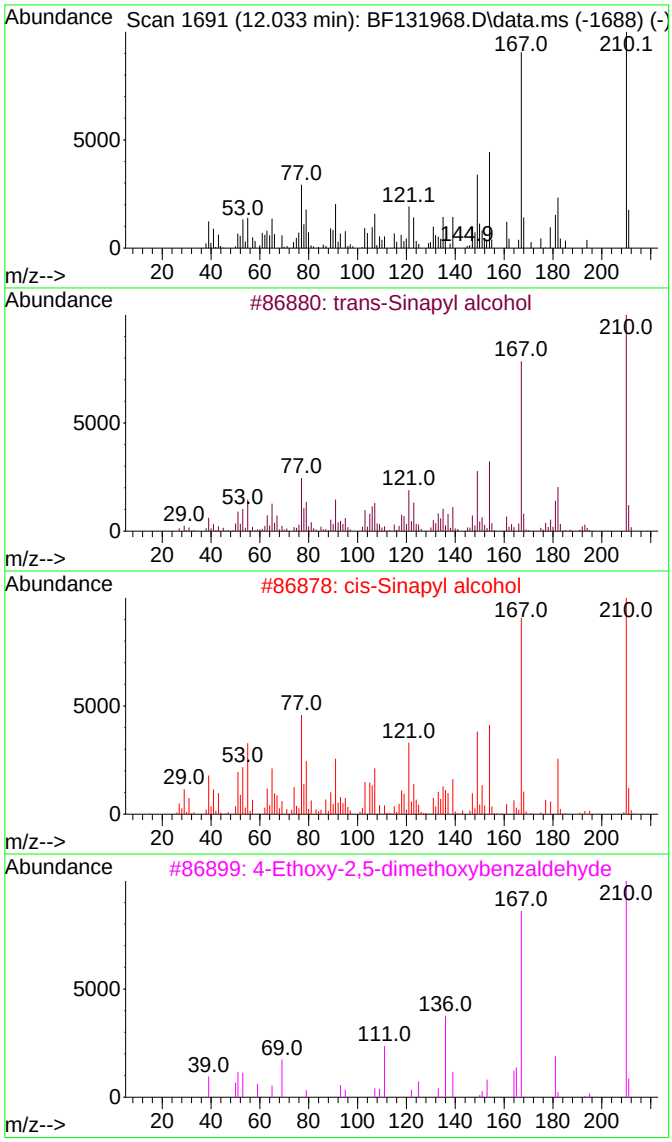
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

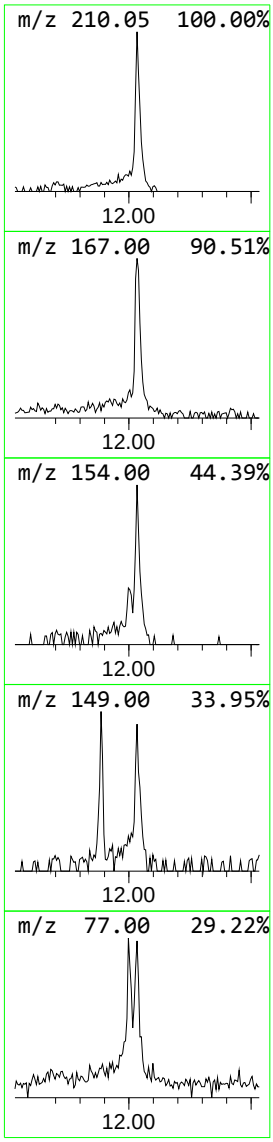
****

Peak Number 6 trans-Sinapyl alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.033	2.74 ng	110883	Phenanthrene-d10	11.327

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	96
2	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	64
3	4-Ethoxy-2,5-dimethoxybenzaldehyde	210	C11H14O4	1000121-30-2	47
4	1H-Naphtho[2,1-b]pyran-1-one, 3-...	210	C14H10O2	005891-82-7	42
5	Phenol, 2-(2-imidazo[1,2-a]pyrid...	210	C13H10N2O	057636-32-5	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131968.D
Acq On : 09 Jan 2023 17:52
Operator : CG\JU
Sample : 01043-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-203

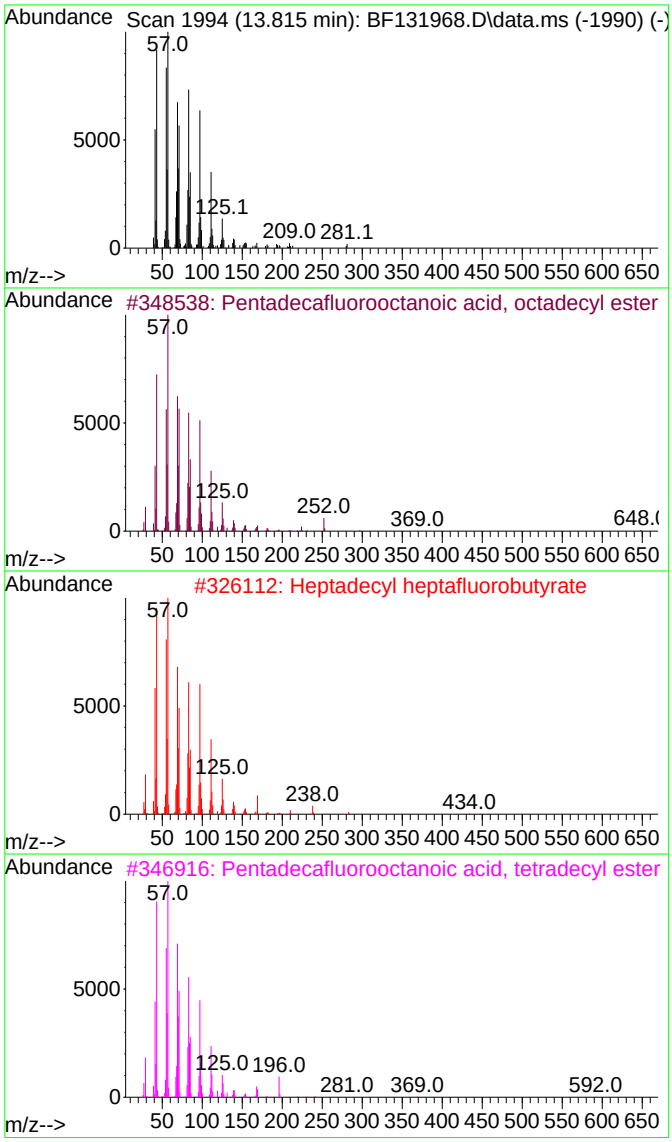
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

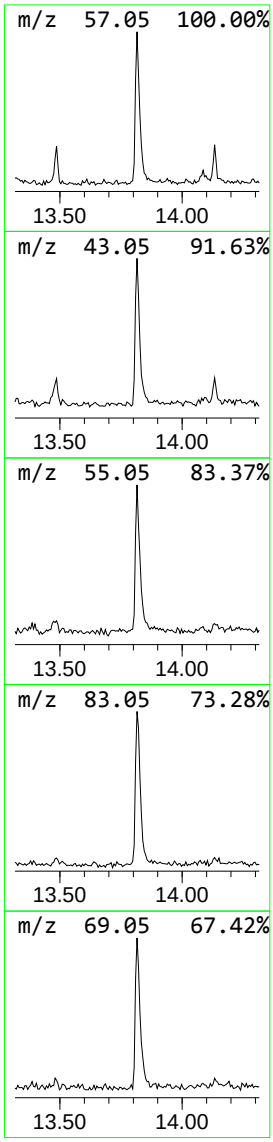
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.815	10.05 ng	247535	Chrysene-d12	13.974

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	Pentadecafluorooctanoic acid, te...	610	C22H29F15O2	1000406-04-4	91
4	1-Hexacosene	364	C26H52	018835-33-1	91
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010923\
Data File : BF131968.D
Acq On : 09 Jan 2023 17:52
Operator : CG\JU
Sample : 01043-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-203

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.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
Propane, 1,1-di...	2.146	3.4	ng	83225	1	6.786	494506	20.0
2-Pentanone, 4-...	4.998	41.8	ng	1032200	1	6.786	494506	20.0
Juglone	9.969	3.6	ng	140724	3	9.833	777284	20.0
Benzophenone	10.551	2.3	ng	88776	3	9.833	777284	20.0
n-Hexadecanoic ...	11.857	4.0	ng	160856	4	11.327	809001	20.0
trans-Sinapyl a...	12.033	2.7	ng	110883	4	11.327	809001	20.0
Pentadecafluoro...	13.815	10.1	ng	247535	5	13.974	492570	20.0