LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134393.D
Acq On : 21 Jul 2023 10:31
Operator : CG\JU
Sample : PB154284BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB154284BL

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134393.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.487	403	408	419	rBV	1194424	1470640	41.40%	6.737%
2	5.104	505	513	525	rBV	1162535	1869306	52.62%	8.564%
3	5.492	574	579	582	rBV	2195348	2121596	59.72%	9.720%
4	5.863	639	642	652	rVB	64515	53324	1.50%	0.244%
5	6.487	742	748	766	rVB	1920411	2167339	61.01%	9.929%
6	6.834	804	807	816	rBV	479151	422750	11.90%	1.937%
7	7.404	899	904	907	rBV	1459651	1394405	39.25%	6.388%
8	8.116	1021	1025	1031	rBV	725222	571086	16.08%	2.616%
9	9.198	1202	1209	1212	rBV	3201431	2874299	80.91%	13.168%
10	9.875	1320	1324	1327	rBV	865620	681175	19.17%	3.121%
11	10.675	1455	1460	1463	rBV	2334065	2162456	60.87%	9.907%
12	11.369	1574	1578	1586	rBV	958755	795937	22.41%	3.646%
13	12.974	1845	1851	1854	rBV	3514564	3552423	100.00%	16.274%
14	14.033	2027	2031	2041	rBV	782296	701150	19.74%	3.212%
15	14.810	2159	2163	2167	rBV	31346	36606	1.03%	0.168%
16	15.157	2218	2222	2227	rBV	39003	49976	1.41%	0.229%
17	15.539	2281	2287	2294	rBV	463234	675818	19.02%	3.096%
18	16.009	2362	2367	2374	rBV2	47417	70056	1.97%	0.321%
19	16.545	2453	2458	2468	rVB2	39205	79192	2.23%	0.363%
20	17.174	2560	2565	2574	rVB5	20497	42806	1.20%	0.196%
21	17.927	2688	2693	2700	rVB6	17204	35875	1.01%	0.164%

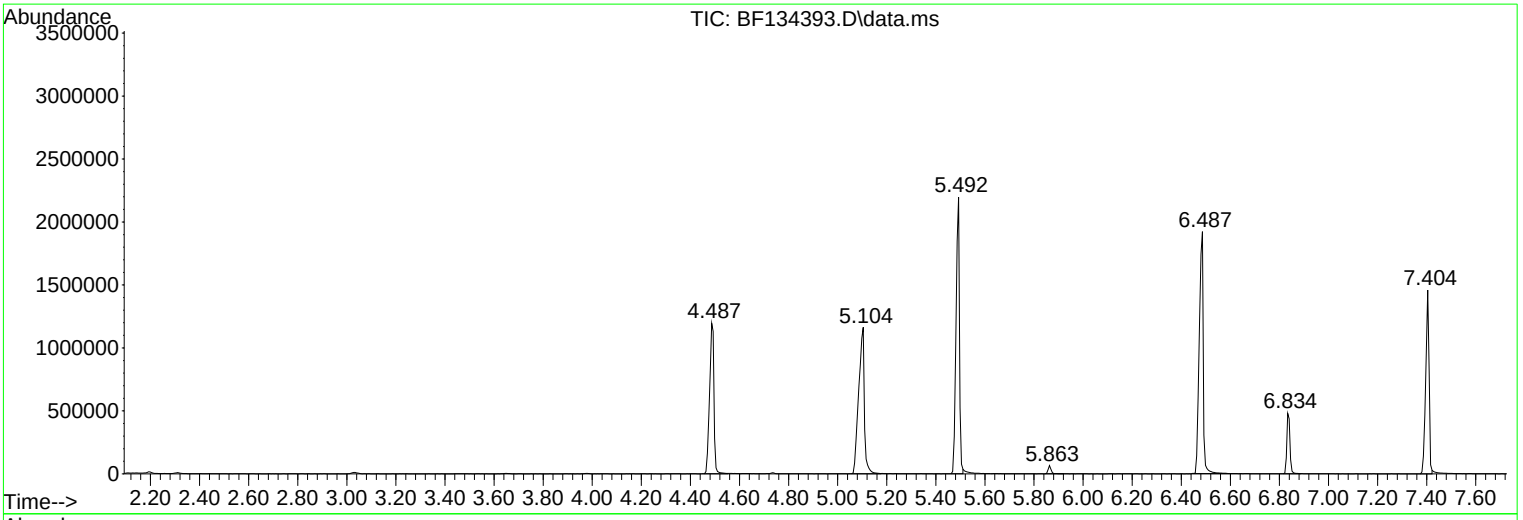
Sum of corrected areas: 21828215

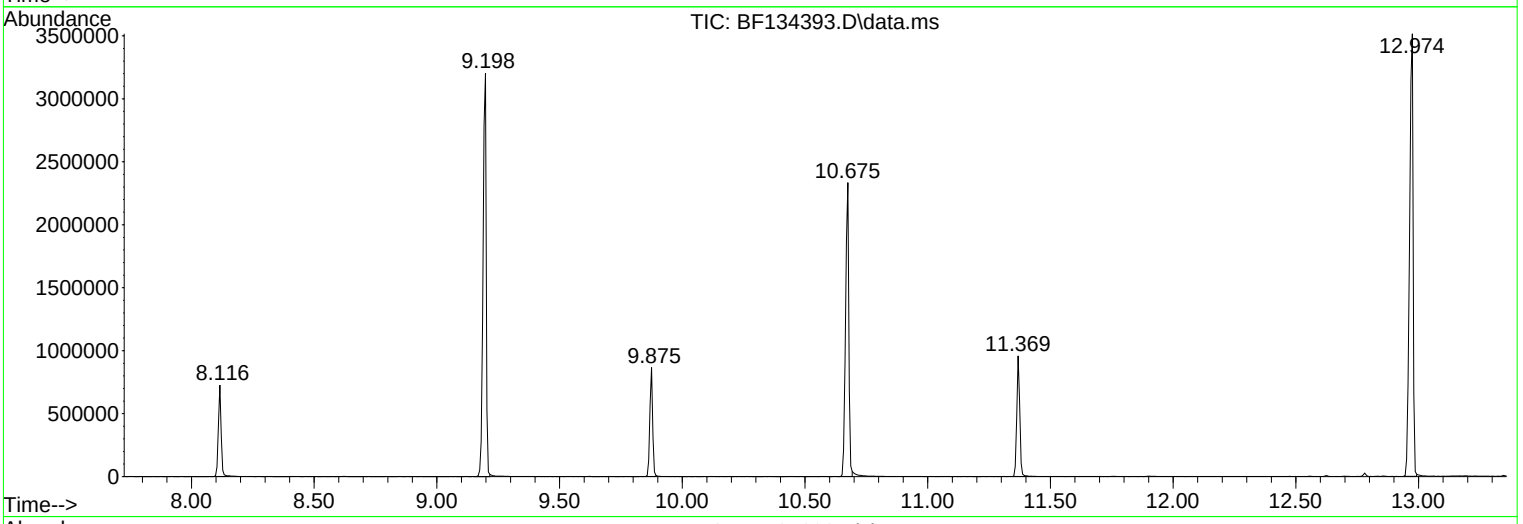
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134393.D
Acq On : 21 Jul 2023 10:31
Operator : CG\JU
Sample : PB154284BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

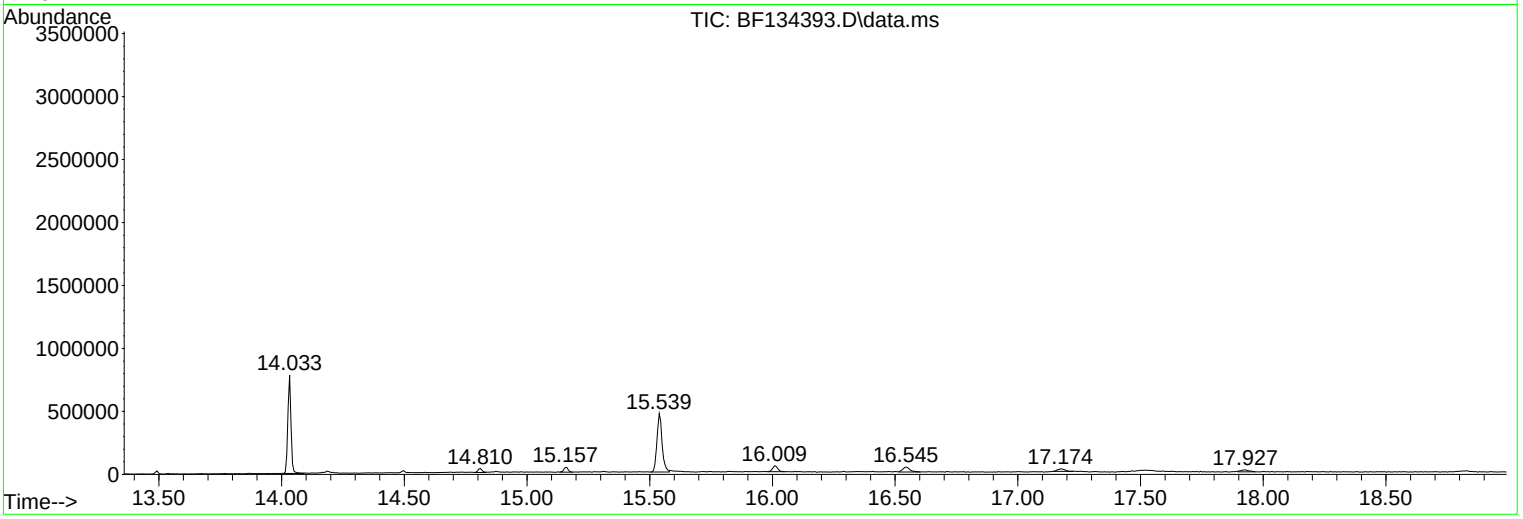
Instrument :
BNA_F
ClientSampleId :
PB154284BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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\BF072123\
Data File : BF134393.D
Acq On : 21 Jul 2023 10:31
Operator : CG\JU
Sample : PB154284BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB154284BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

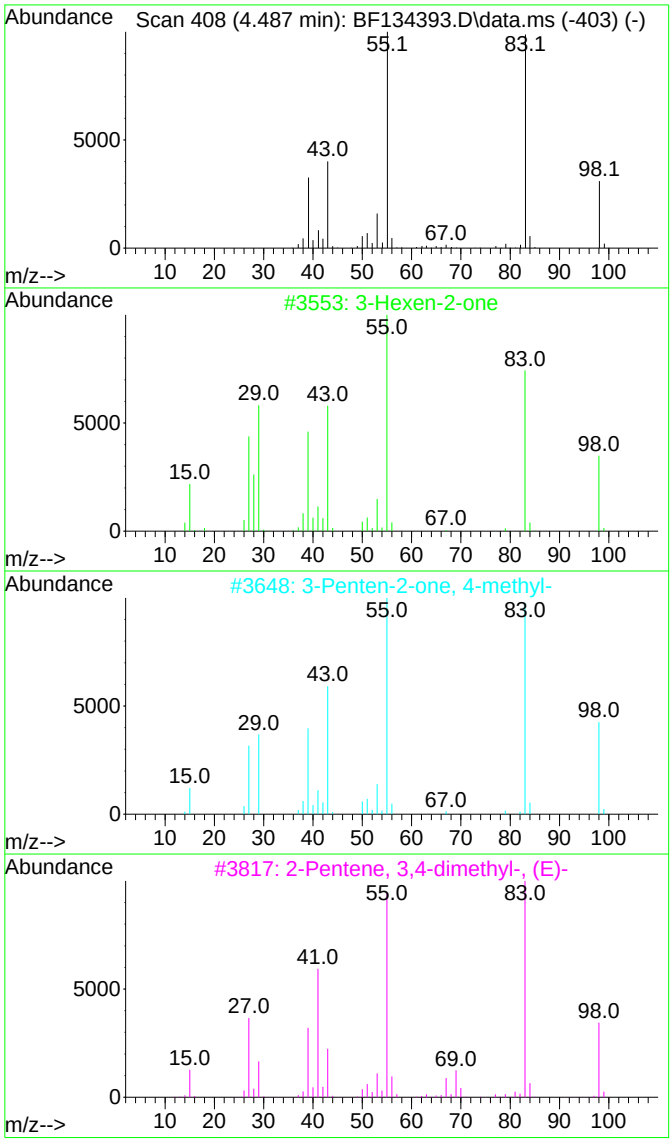
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

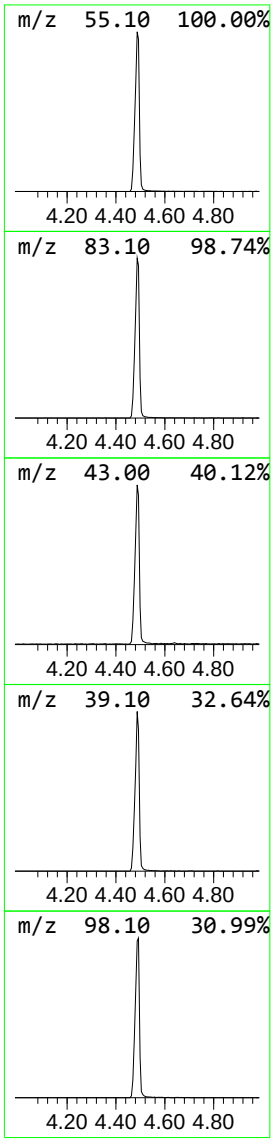
****

Peak Number 1 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.487	69.57 ng	1470640	1,4-Dichlorobenzene-d4	6.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134393.D
Acq On : 21 Jul 2023 10:31
Operator : CG\JU
Sample : PB154284BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB154284BL

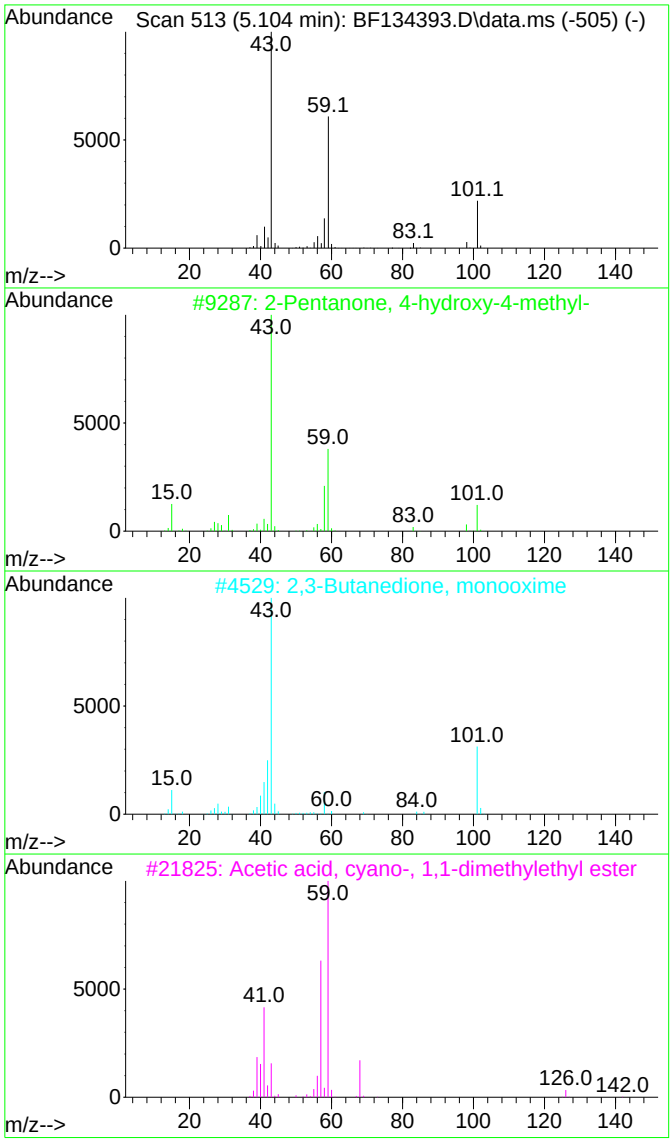
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

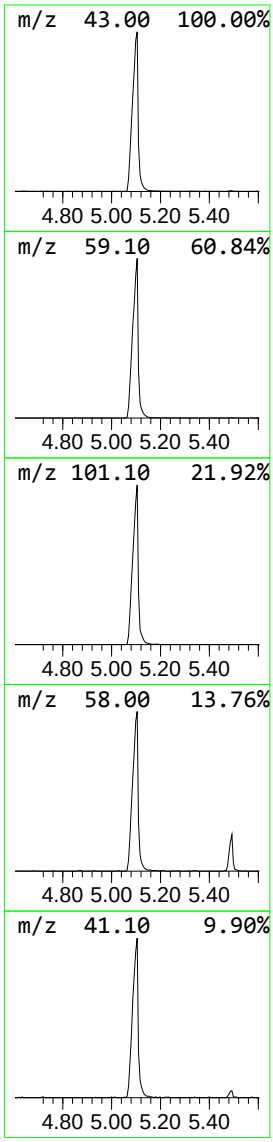
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	88.44 ng	1869310	1,4-Dichlorobenzene-d4	6.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
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	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134393.D
Acq On : 21 Jul 2023 10:31
Operator : CG\JU
Sample : PB154284BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB154284BL

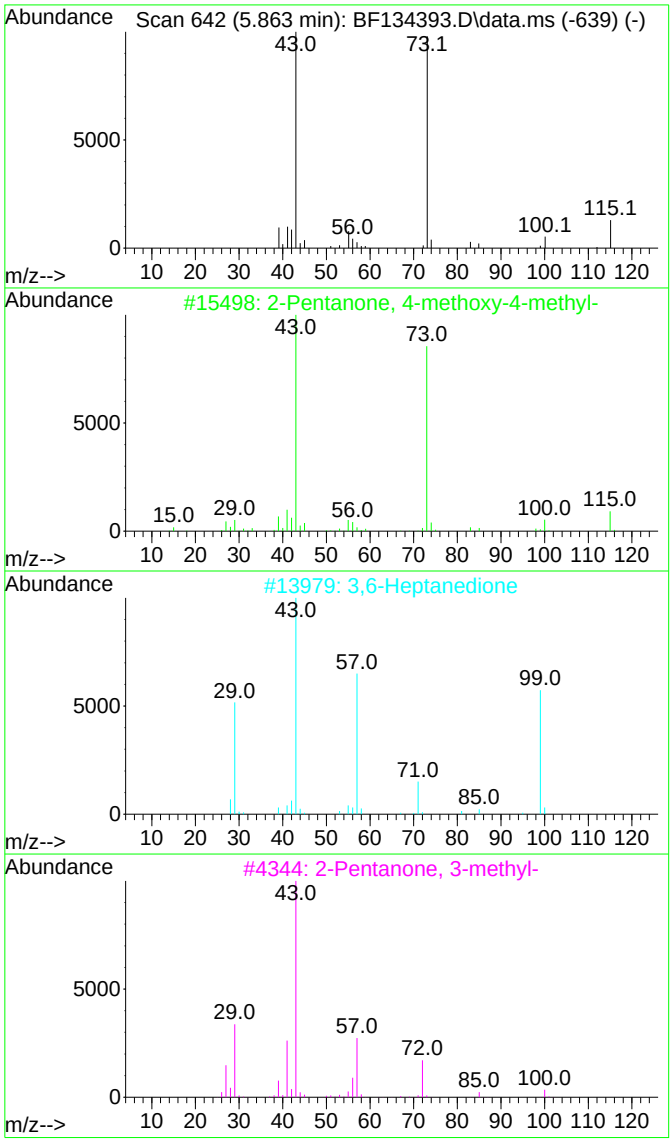
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

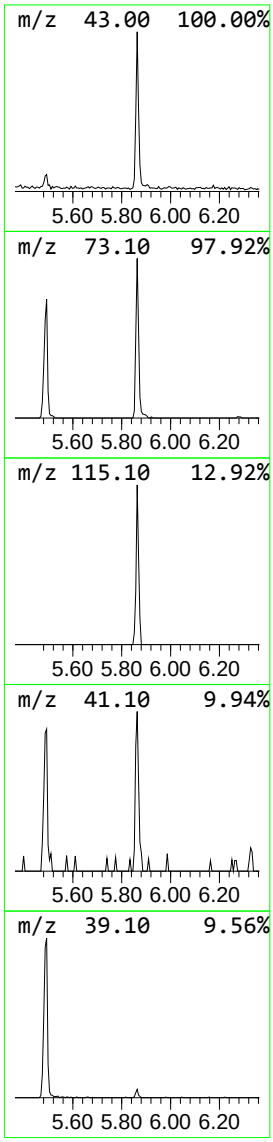
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.863	2.52 ng	53324	1,4-Dichlorobenzene-d4	6.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2	3,6-Heptanedione	128	C7H12O2	001703-51-1	23
3	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
4	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	10
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134393.D
Acq On : 21 Jul 2023 10:31
Operator : CG\JU
Sample : PB154284BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB154284BL

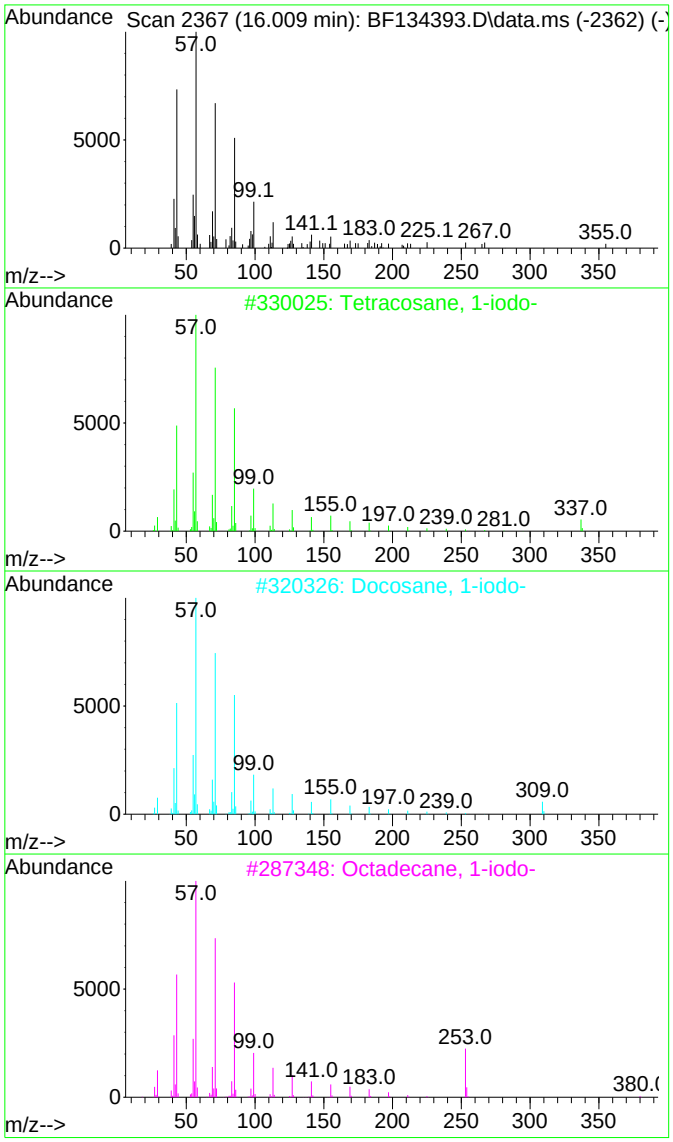
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

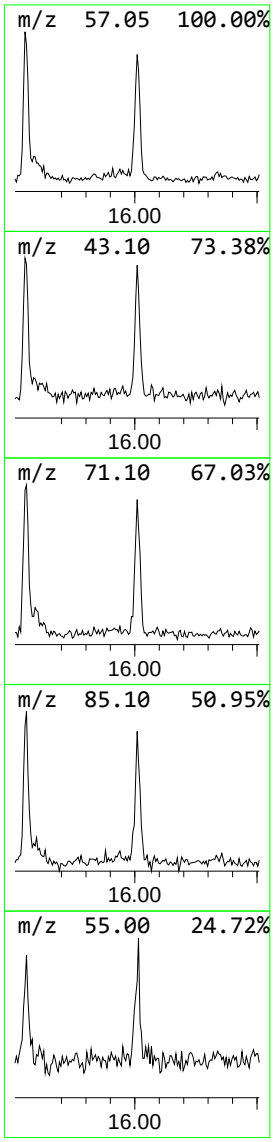
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Tetracosane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.009	2.07 ng	70056	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	87
2	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
4	Octacosane	394	C28H58	000630-02-4	83
5	Hexacosane	366	C26H54	000630-01-3	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134393.D
Acq On : 21 Jul 2023 10:31
Operator : CG\JU
Sample : PB154284BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB154284BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

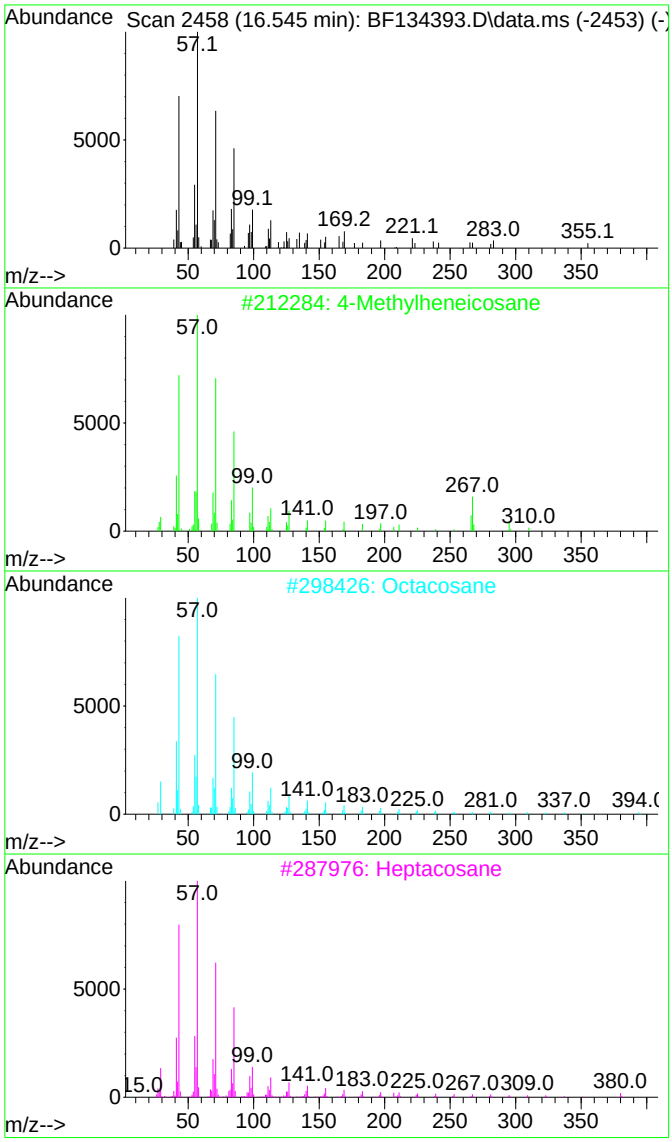
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

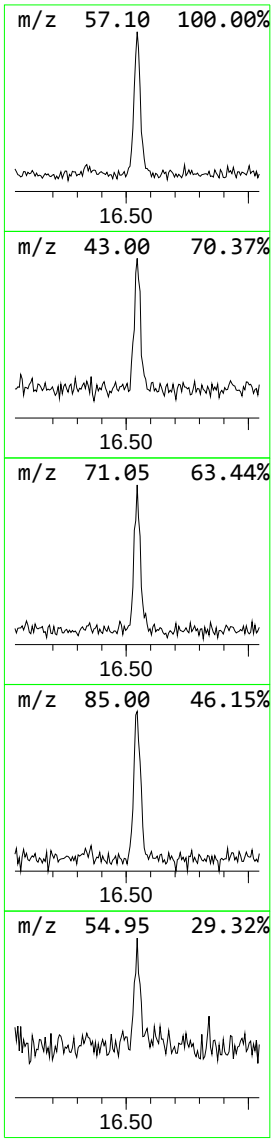
****

Peak Number 5 4-Methylheneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.545	2.34 ng	79192	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methylheneicosane	310	C22H46	025117-29-7	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Heptacosane	380	C27H56	000593-49-7	87
4	Hentriacontane	437	C31H64	000630-04-6	87
5	Hexacosane	366	C26H54	000630-01-3	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072123\
Data File : BF134393.D
Acq On : 21 Jul 2023 10:31
Operator : CG\JU
Sample : PB154284BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB154284BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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
3-Hexen-2-one	4.487	69.6	ng	1470640	1	6.839	422750	20.0
2-Pentanone, 4-...	5.104	88.4	ng	1869310	1	6.839	422750	20.0
2-Pentanone, 4-...	5.863	2.5	ng	53324	1	6.839	422750	20.0
Tetracosane, 1-...	16.009	2.1	ng	70056	6	15.539	675818	20.0
4-Methylheneico...	16.545	2.3	ng	79192	6	15.539	675818	20.0