LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139294.D
Acq On : 10 Sep 2024 12:20
Operator : RC/JU
Sample : PB163252BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163252BL

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-BF090424.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139294.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.287	25	33	41	rVB	91900	156945	2.73%	0.417%
2	5.140	510	518	529	rBV	194793	369169	6.42%	0.981%
3	5.522	575	583	588	rBV	3281589	4894269	85.12%	13.008%
4	6.516	744	752	757	rBV	3160933	4962723	86.31%	13.190%
5	6.887	810	815	820	rVB	905152	1101756	19.16%	2.928%
6	7.451	903	911	916	rBV	2159582	3289806	57.21%	8.744%
7	8.169	1026	1033	1038	rBV	1069288	1436250	24.98%	3.817%
8	9.245	1208	1216	1222	rBV	3914138	5702718	99.18%	15.157%
9	9.928	1324	1332	1337	rBV	1211578	1628201	28.32%	4.328%
10	10.716	1458	1466	1471	rBV	2507000	3468332	60.32%	9.218%
11	11.410	1578	1584	1590	rBV	1345754	1740688	30.27%	4.627%
12	13.004	1848	1855	1860	rBV	4204632	5750127	100.00%	15.283%
13	14.051	2027	2033	2050	rVB	1026042	1309770	22.78%	3.481%
14	14.833	2161	2166	2172	rBV	47005	61962	1.08%	0.165%
15	15.180	2220	2225	2230	rVB	62741	86989	1.51%	0.231%
16	15.527	2278	2284	2288	rBV	599803	916638	15.94%	2.436%
17	15.562	2288	2290	2301	rVB	87569	132535	2.30%	0.352%
18	16.015	2360	2367	2382	rVB	72781	132401	2.30%	0.352%
19	16.527	2448	2454	2469	rVB	74057	146997	2.56%	0.391%
20	17.139	2550	2558	2572	rBV2	56494	157967	2.75%	0.420%
21	17.856	2672	2680	2695	rVB	40928	112369	1.95%	0.299%
22	18.715	2818	2826	2838	rVB3	21067	65275	1.14%	0.173%

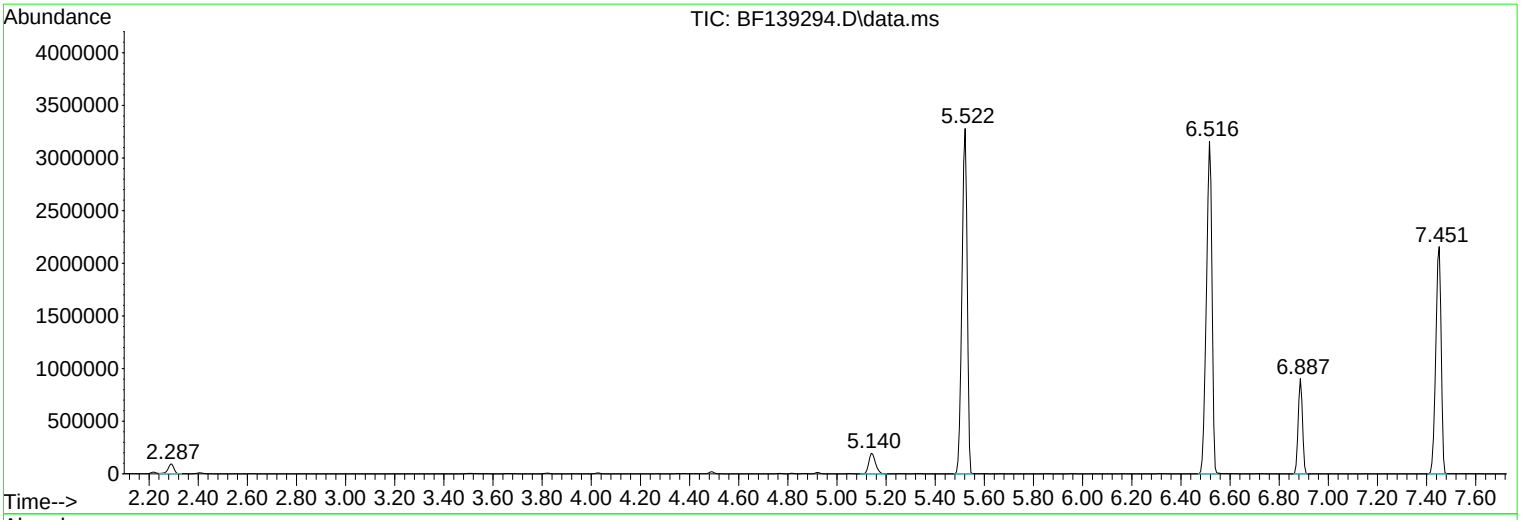
Sum of corrected areas: 37623887

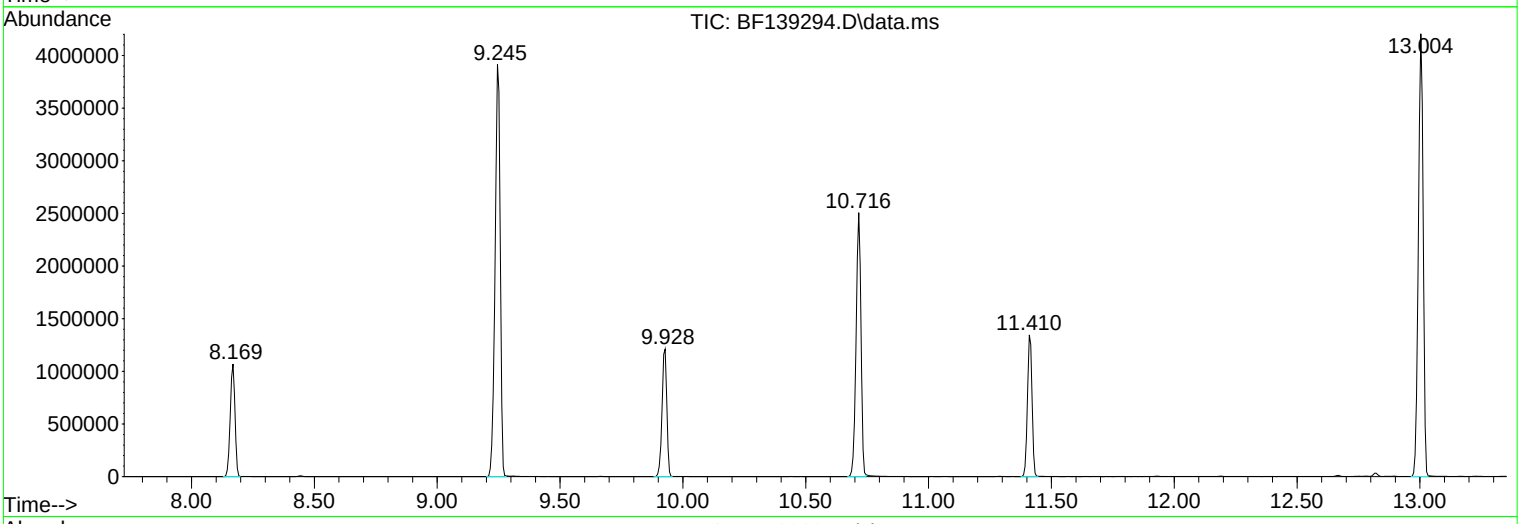
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139294.D
Acq On : 10 Sep 2024 12:20
Operator : RC/JU
Sample : PB163252BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

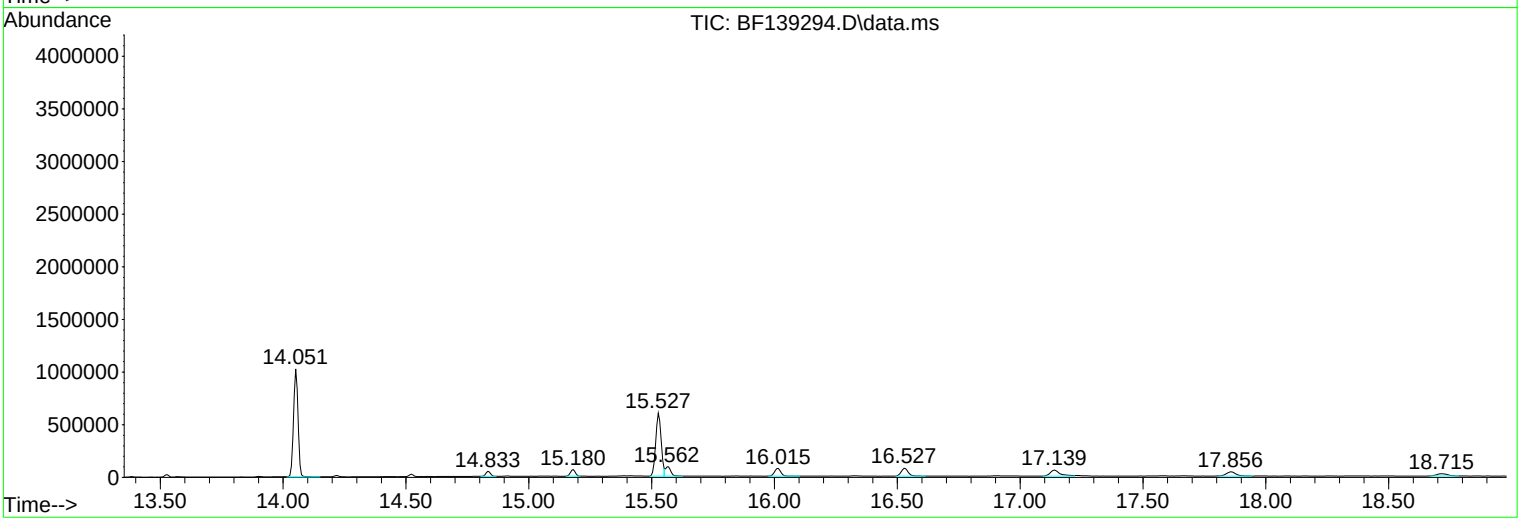
Instrument :
BNA_F
ClientSampleId :
PB163252BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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\BF091024\
Data File : BF139294.D
Acq On : 10 Sep 2024 12:20
Operator : RC/JU
Sample : PB163252BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163252BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

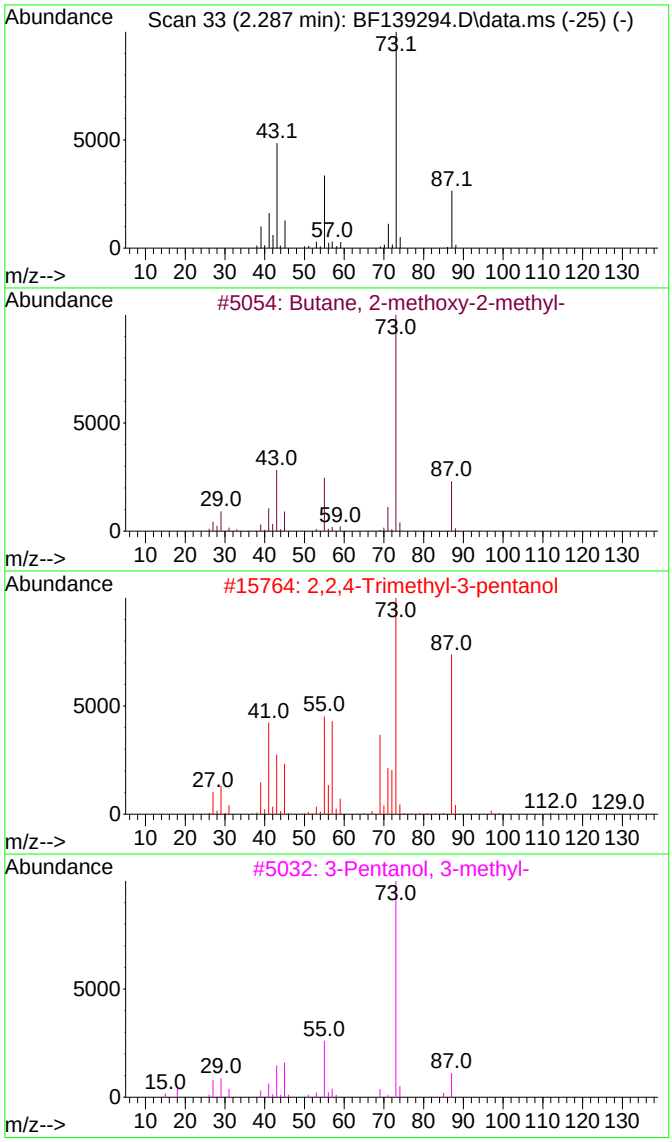
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

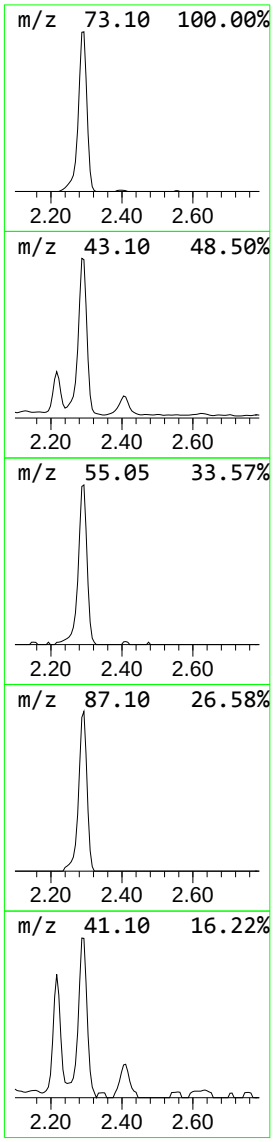
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	2.85 ng	156945	1,4-Dichlorobenzene-d4	6.887

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	39
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	32
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139294.D
Acq On : 10 Sep 2024 12:20
Operator : RC/JU
Sample : PB163252BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163252BL

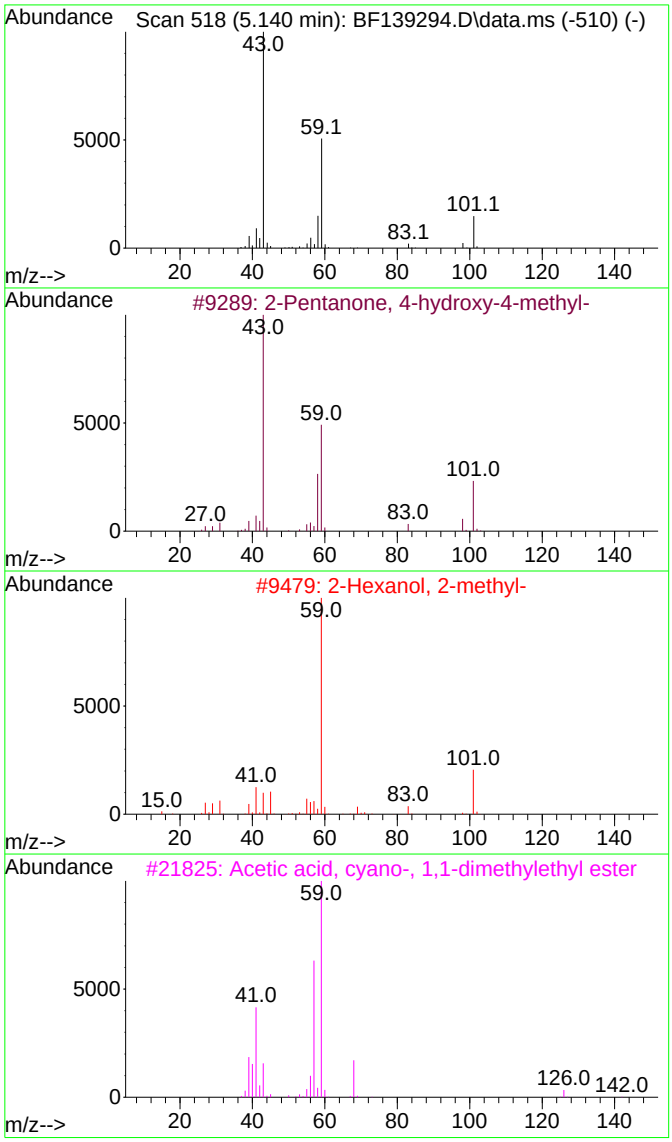
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

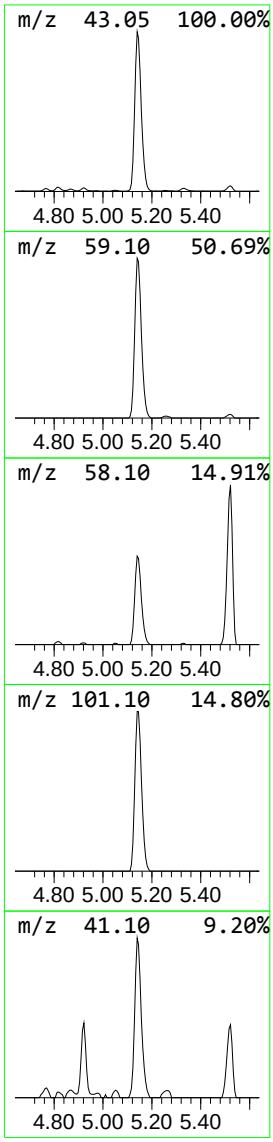
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.140	6.70 ng	369169	1,4-Dichlorobenzene-d4	6.887

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139294.D
Acq On : 10 Sep 2024 12:20
Operator : RC/JU
Sample : PB163252BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163252BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

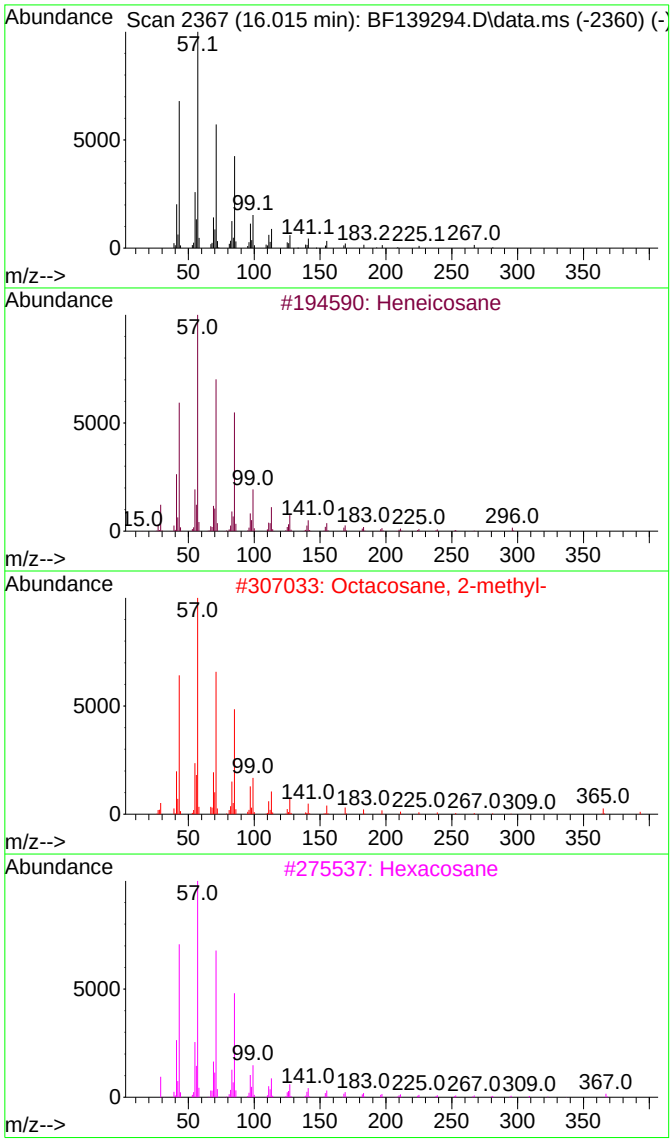
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

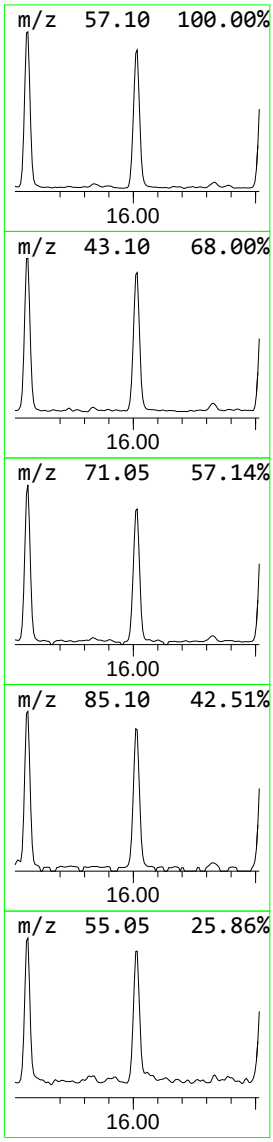
****

Peak Number 3 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.015	2.89 ng	132401	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139294.D
Acq On : 10 Sep 2024 12:20
Operator : RC/JU
Sample : PB163252BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163252BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

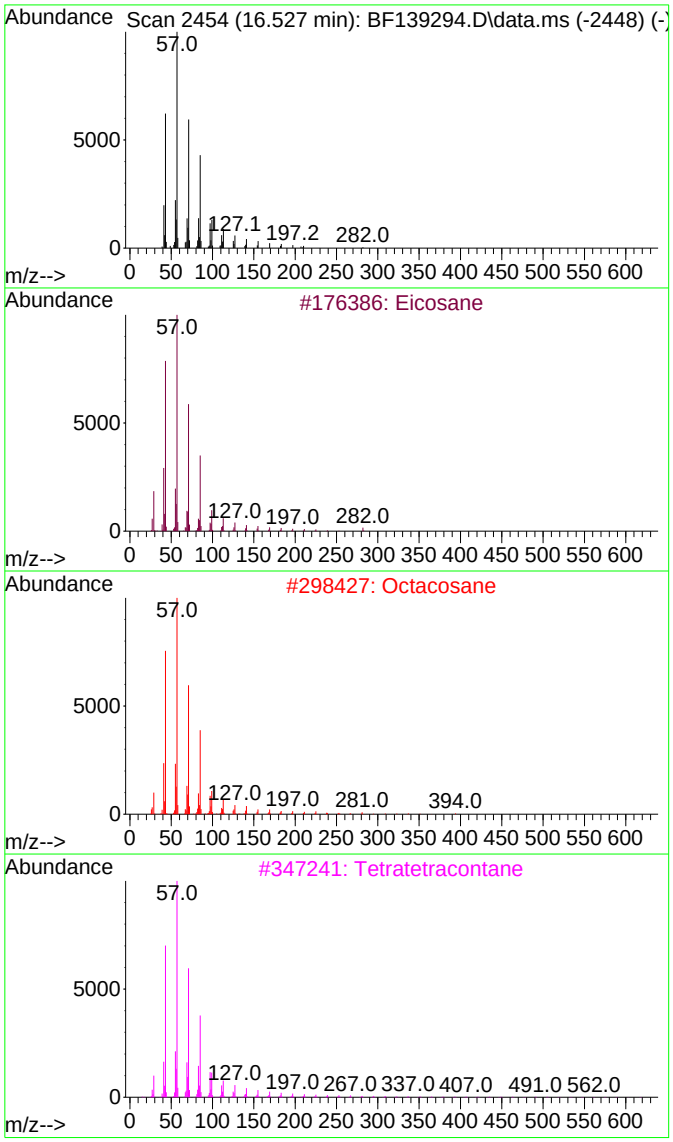
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

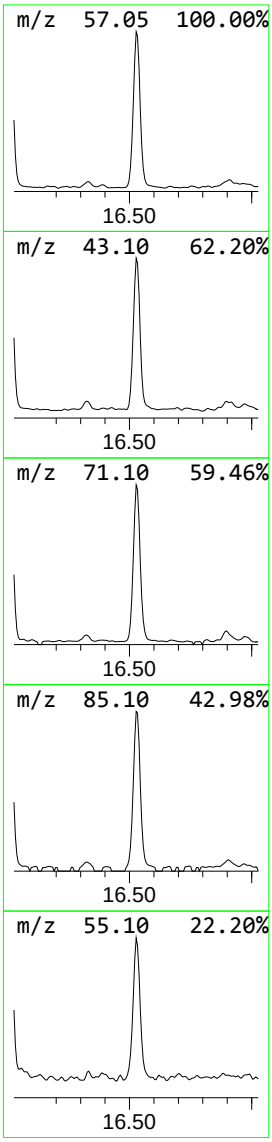
****

Peak Number 4 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.527	3.21 ng	146997	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Octacosane	394	C28H58	000630-02-4	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Hentriacontane	437	C31H64	000630-04-6	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139294.D
Acq On : 10 Sep 2024 12:20
Operator : RC/JU
Sample : PB163252BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163252BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

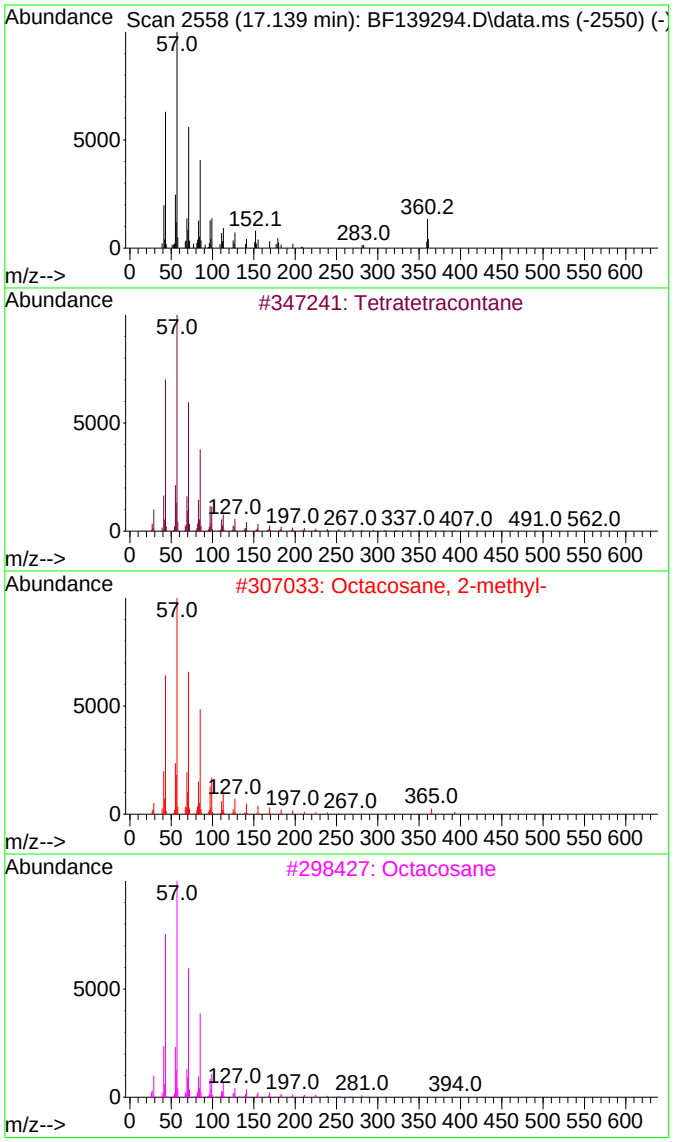
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

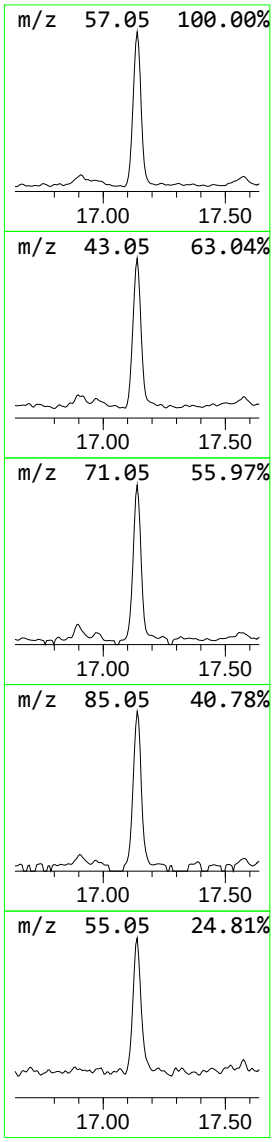
****

Peak Number 5 Tetratetracontane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.139	3.45 ng	157967	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	87
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Heptacosane	380	C27H56	000593-49-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139294.D
Acq On : 10 Sep 2024 12:20
Operator : RC/JU
Sample : PB163252BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163252BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

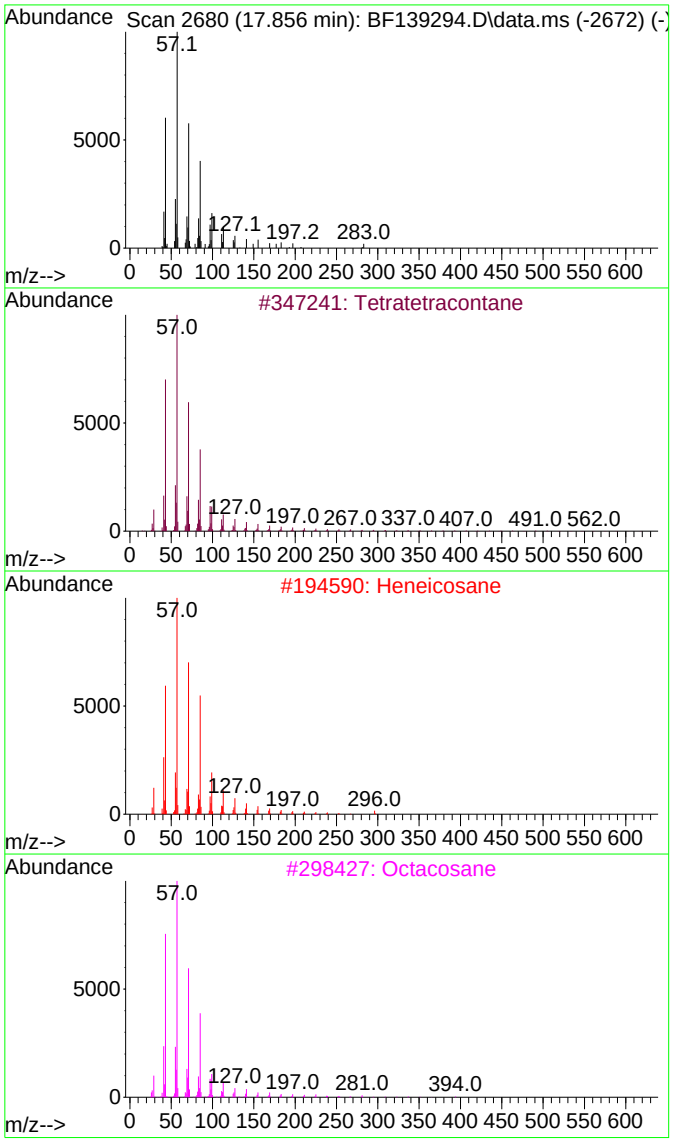
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

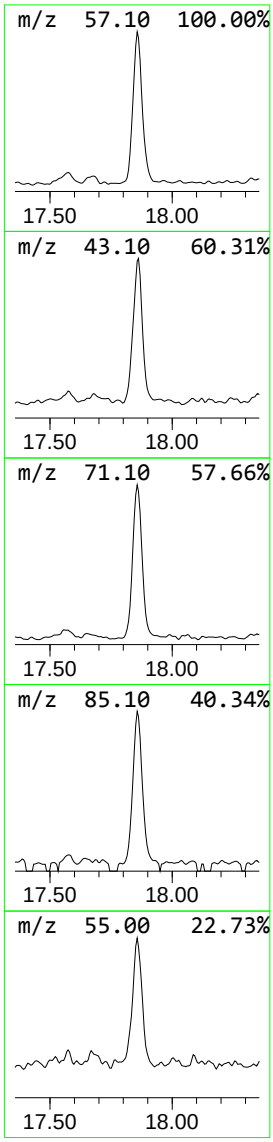
****

Peak Number 6 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.856	2.45 ng	112369	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Pentacosane	352	C25H52	000629-99-2	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091024\
Data File : BF139294.D
Acq On : 10 Sep 2024 12:20
Operator : RC/JU
Sample : PB163252BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163252BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.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...	2.287	2.9	ng	156945	1	6.887	1101760	20.0
2-Pentanone, 4-...	5.140	6.7	ng	369169	1	6.887	1101760	20.0
Heneicosane	16.015	2.9	ng	132401	6	15.527	916638	20.0
Eicosane	16.527	3.2	ng	146997	6	15.527	916638	20.0
Tetratetracontane	17.139	3.5	ng	157967	6	15.527	916638	20.0
Octacosane	17.856	2.5	ng	112369	6	15.527	916638	20.0