LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090924\
Data File : BF139281.D
Acq On : 09 Sep 2024 14:15
Operator : RC/JU
Sample : PB163214BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163214BL

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: BF139281.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.246	17	26	34	rVB	86176	145160	2.83%	0.431%
2	5.134	506	517	530	rVB	187554	344750	6.71%	1.023%
3	5.516	575	582	587	rBV	3175672	4570594	89.00%	13.558%
4	6.516	744	752	757	rBV	3013516	4654750	90.64%	13.807%
5	6.887	810	815	820	rBV	847011	1017284	19.81%	3.018%
6	7.451	903	911	916	rBV	2096958	3049471	59.38%	9.046%
7	8.169	1027	1033	1038	rBV	1040132	1320648	25.72%	3.917%
8	9.245	1209	1216	1221	rBV	3760697	5135500	100.00%	15.233%
9	9.922	1325	1331	1337	rBV	1138934	1470034	28.62%	4.361%
10	10.716	1459	1466	1471	rBV	2243719	3041194	59.22%	9.021%
11	11.410	1579	1584	1589	rBV	1232105	1532788	29.85%	4.547%
12	13.004	1848	1855	1860	rBV	3493331	4888892	95.20%	14.502%
13	14.051	2027	2033	2044	rBV	767068	1021087	19.88%	3.029%
14	15.180	2220	2225	2230	rBV	44944	66468	1.29%	0.197%
15	15.527	2277	2284	2288	rBV	476448	749466	14.59%	2.223%
16	15.562	2288	2290	2302	rVB	72030	109349	2.13%	0.324%
17	16.010	2360	2366	2374	rBV	74485	133796	2.61%	0.397%
18	16.527	2448	2454	2464	rBV	77177	152174	2.96%	0.451%
19	17.139	2551	2558	2566	rBV	53803	117391	2.29%	0.348%
20	17.856	2673	2680	2695	rVB	41149	116255	2.26%	0.345%
21	18.715	2818	2826	2840	rVB2	23993	75362	1.47%	0.224%

Sum of corrected areas: 33712413

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090924\
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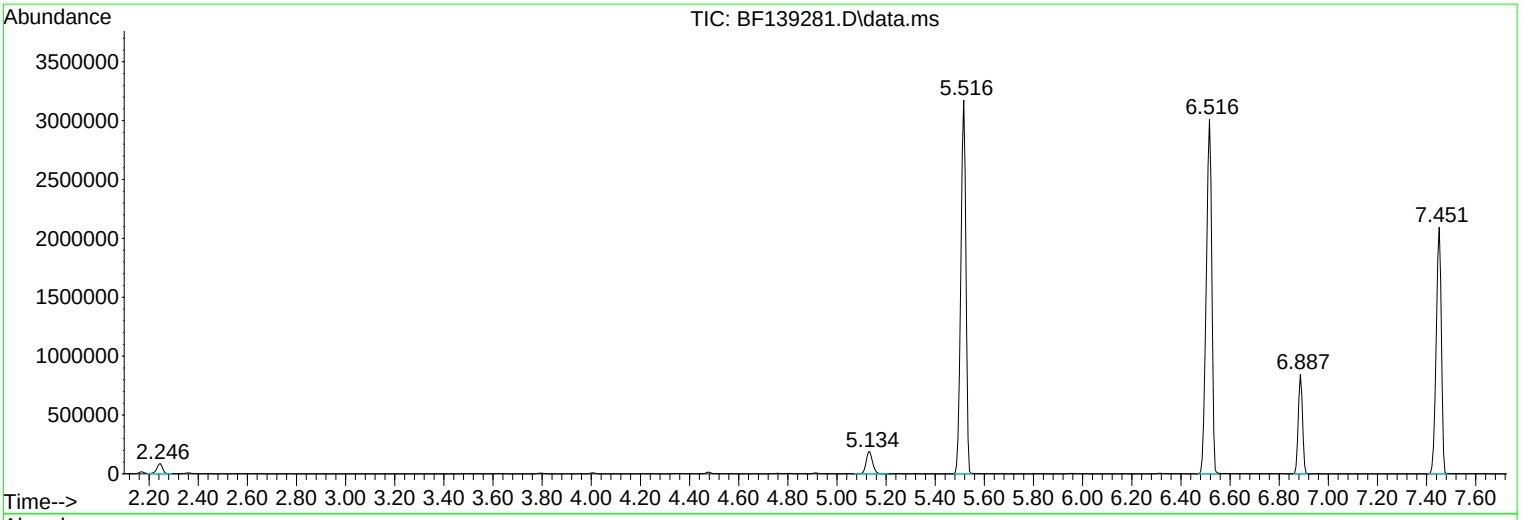
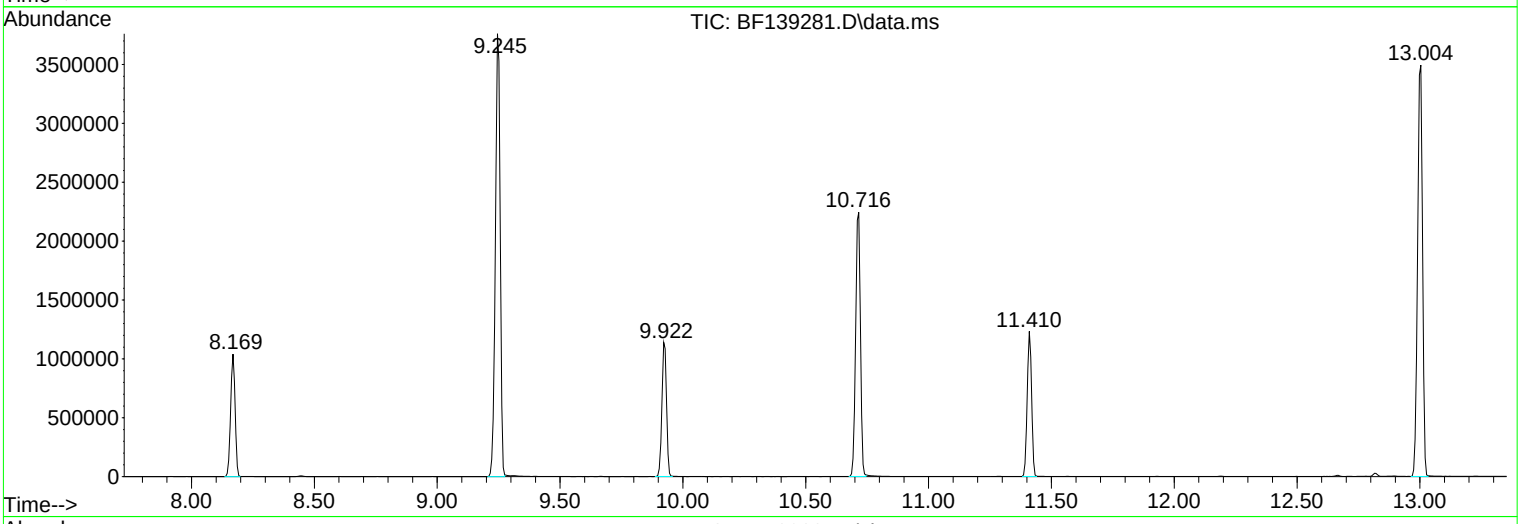
Misc :
ALS Vial : 3 Sample Multiplier: 1

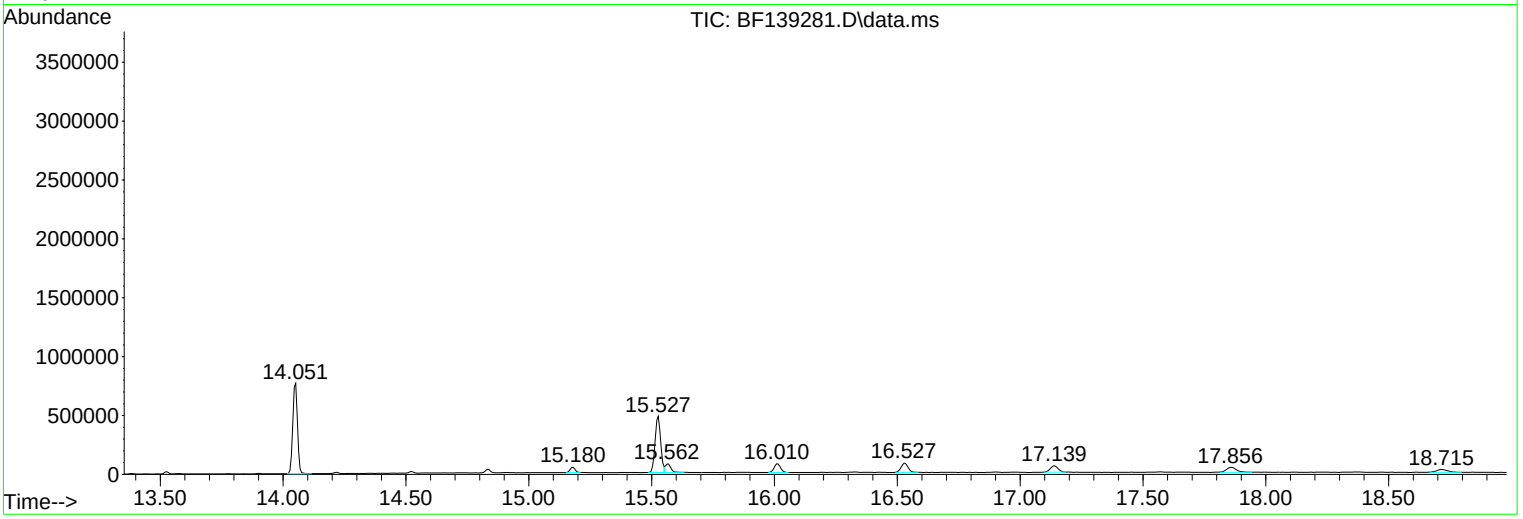
Instrument :
BNA_F
ClientSampleId :
PB163214BL

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\BF090924\
Data File : BF139281.D
Acq On : 09 Sep 2024 14:15
Operator : RC/JU
Sample : PB163214BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB163214BL

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

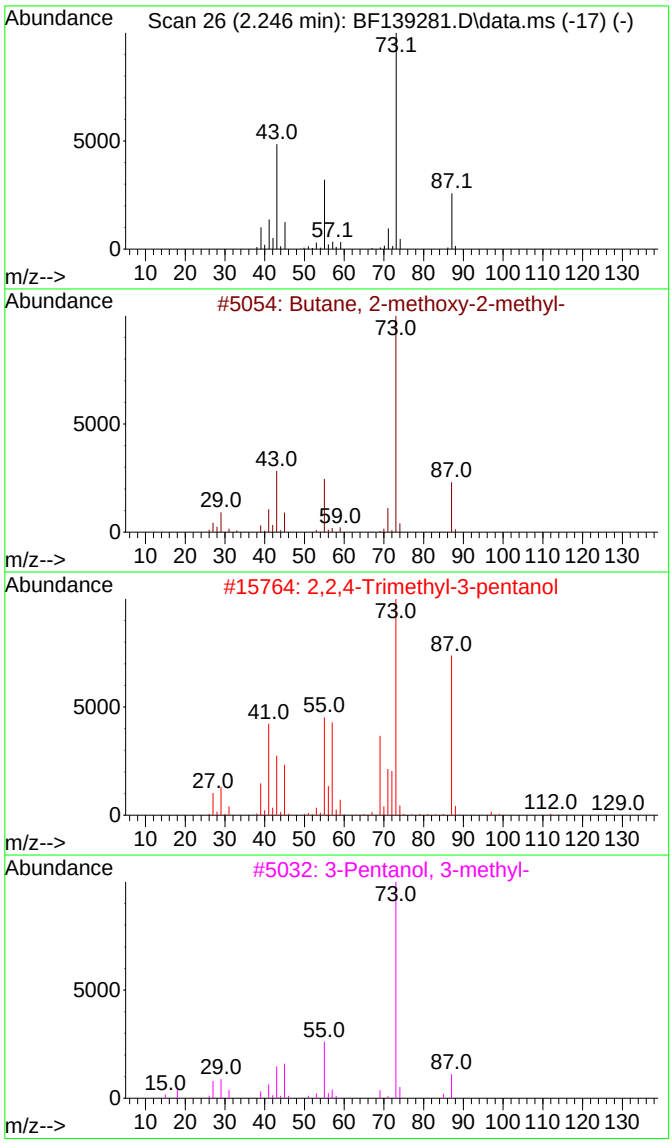
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

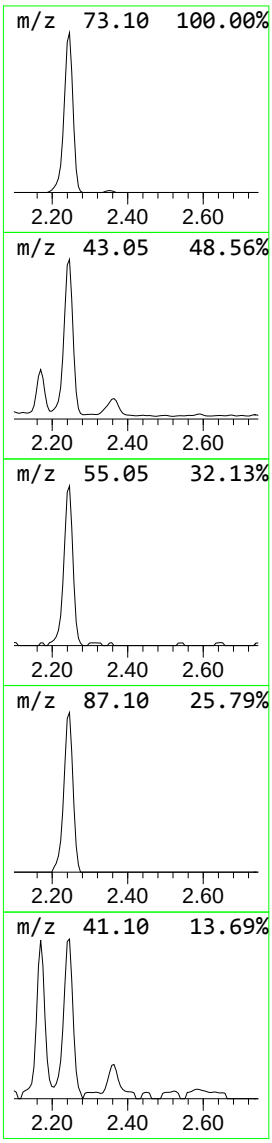
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.246	2.85 ng	145160	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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17





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Sample : PB163214BL
Misc :
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Instrument :
BNA_F
ClientSampleId :
PB163214BL

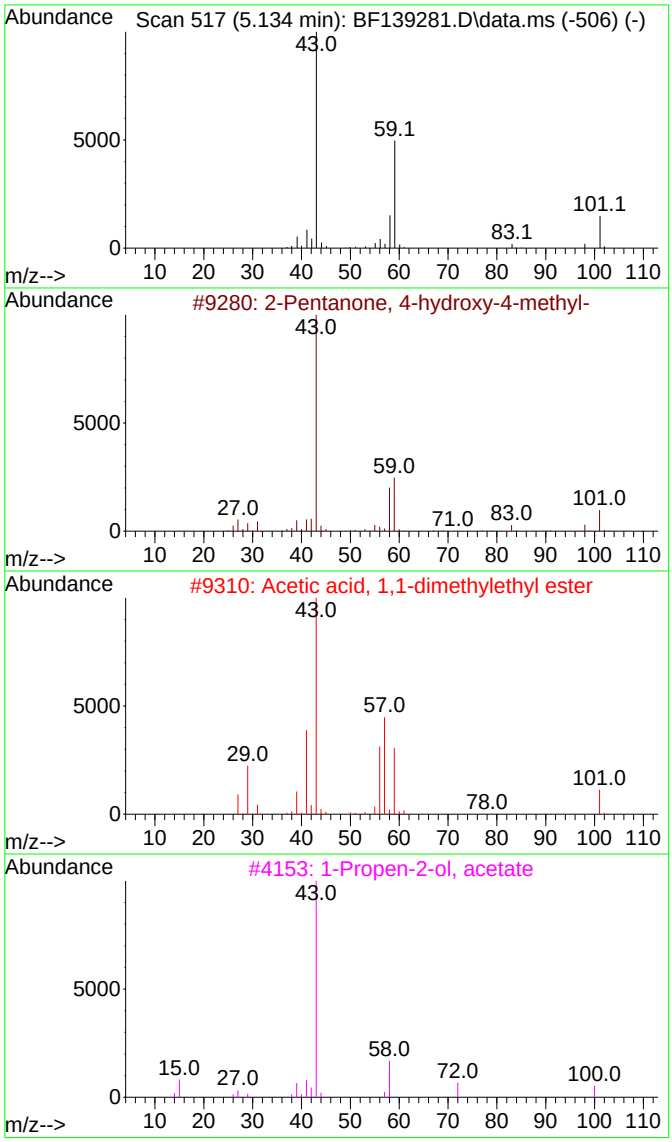
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

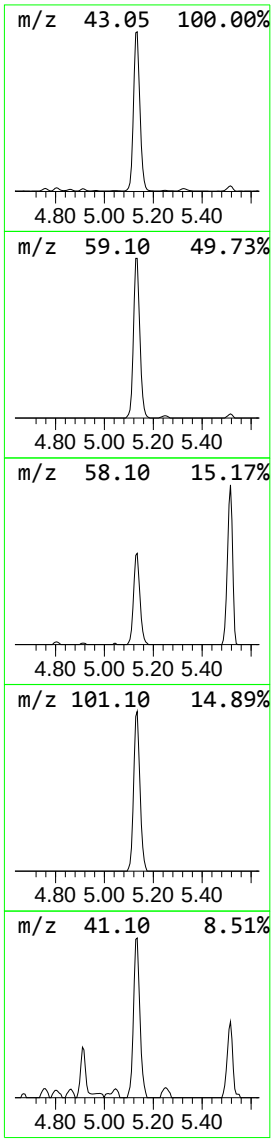
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.134	6.78 ng	344750	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	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090924\
Data File : BF139281.D
Acq On : 09 Sep 2024 14:15
Operator : RC/JU
Sample : PB163214BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163214BL

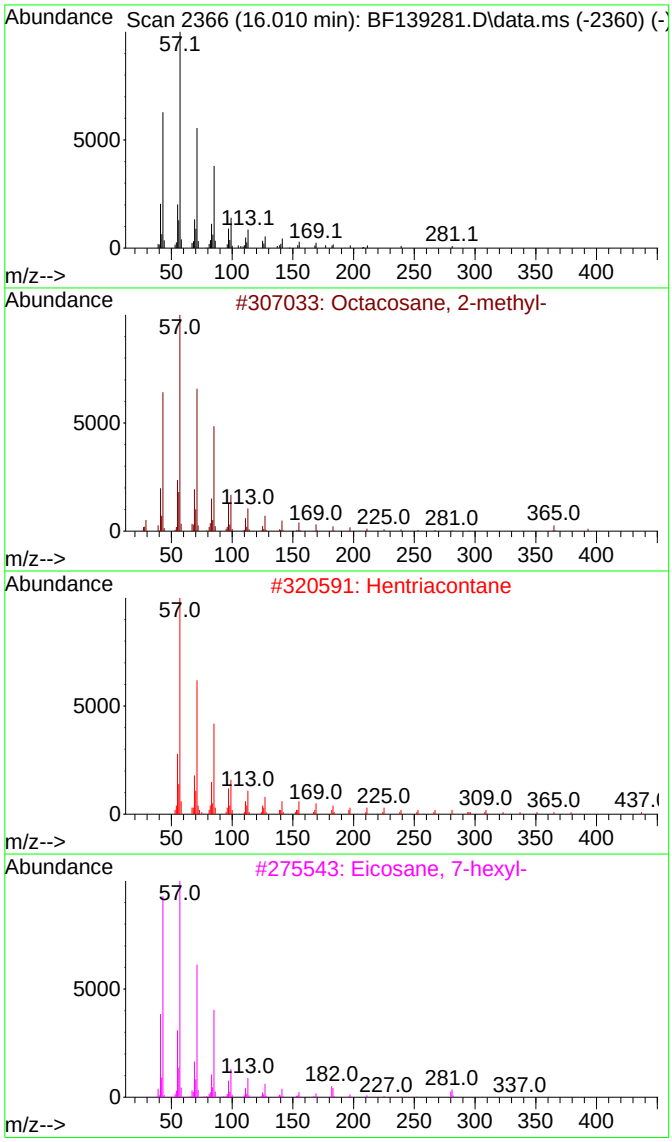
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

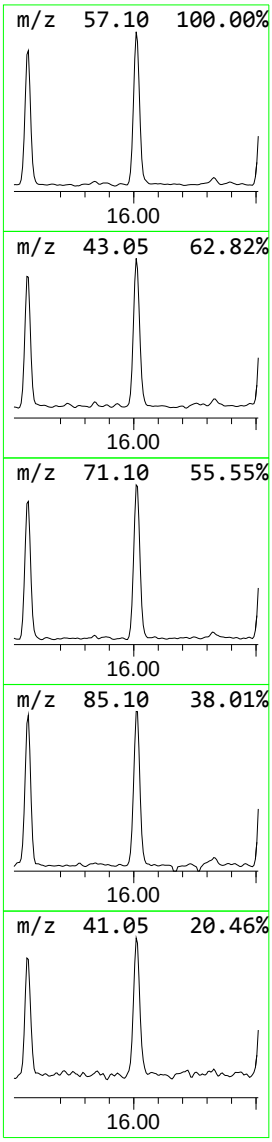
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Octacosane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.009	3.57 ng	133796	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Data File : BF139281.D
Acq On : 09 Sep 2024 14:15
Operator : RC/JU
Sample : PB163214BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163214BL

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

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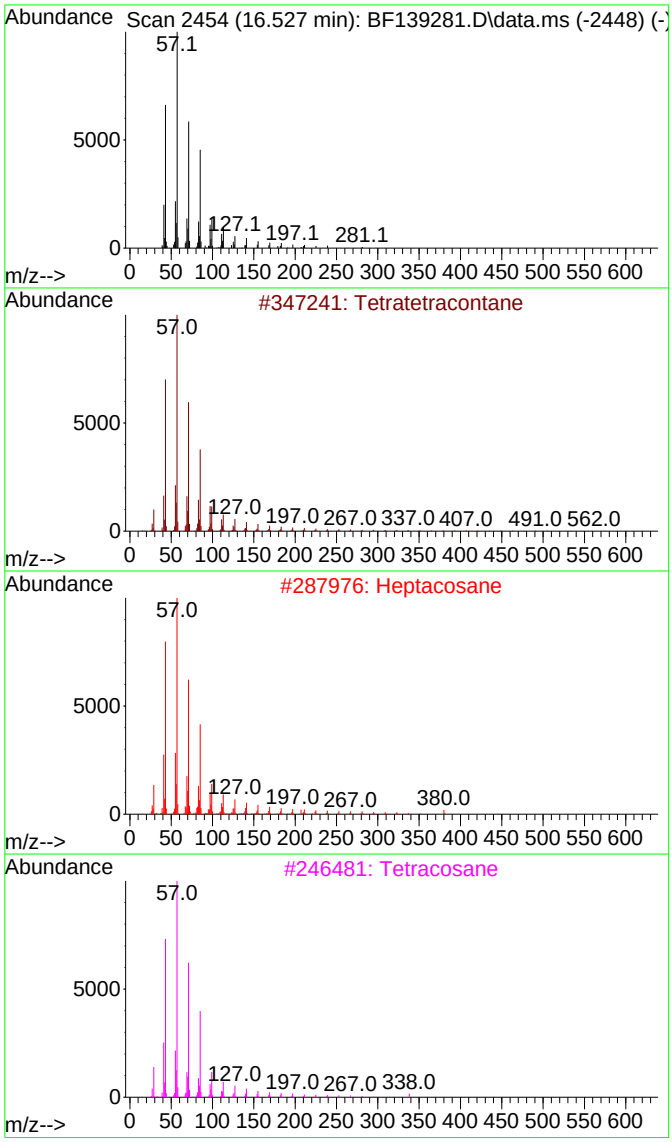
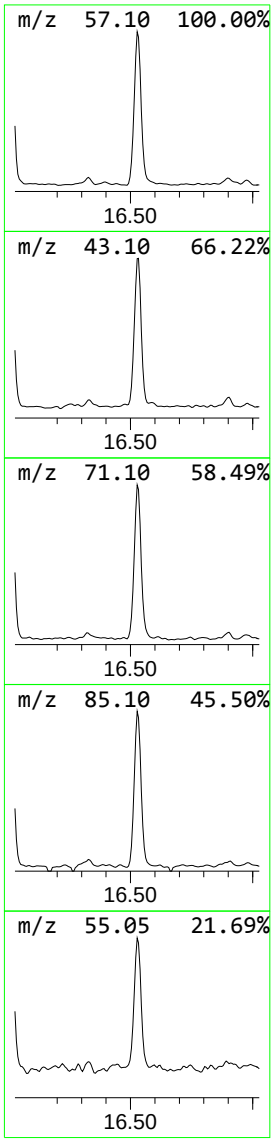
Peak Number 4 Tetratetracontane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.527	4.06 ng	152174	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Octacosane	394	C28H58	000630-02-4	91
5	Heneicosane	296	C21H44	000629-94-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090924\
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Sample : PB163214BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163214BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF090424.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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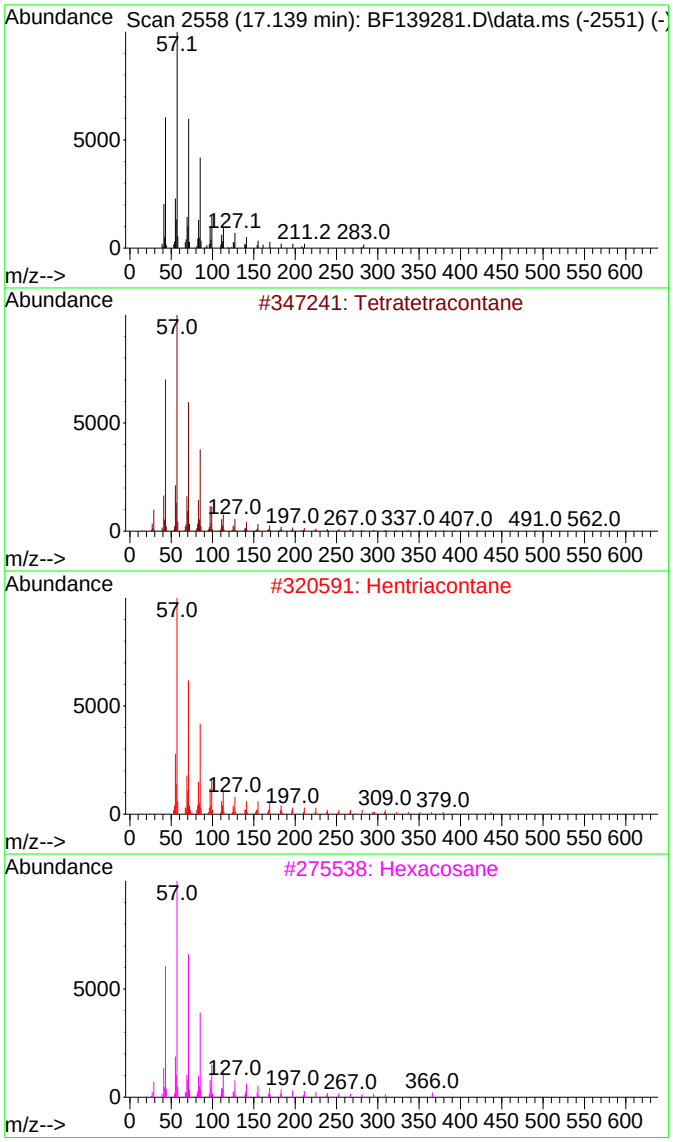
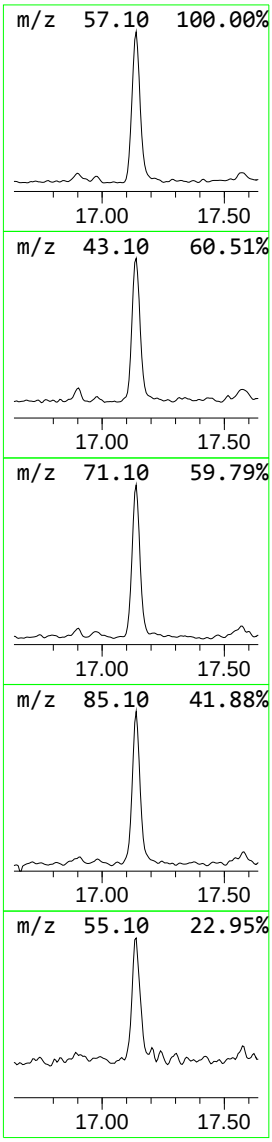
Peak Number 5 Hentriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.139	3.13 ng	117391	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Acq On : 09 Sep 2024 14:15
Operator : RC/JU
Sample : PB163214BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163214BL

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

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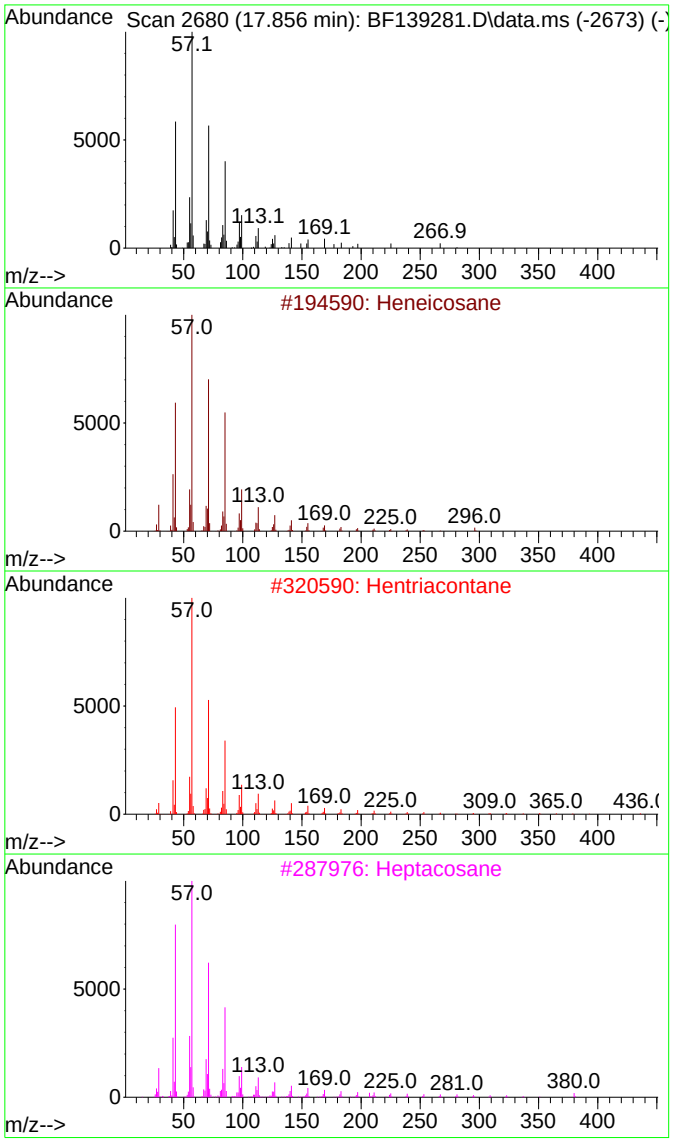
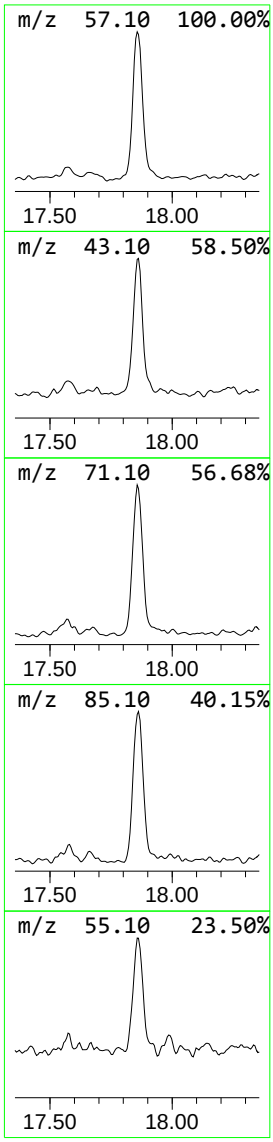
Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.857	3.10 ng	116255	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Hexacosane	366	C26H54	000630-01-3	91





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Acq On : 09 Sep 2024 14:15
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Sample : PB163214BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163214BL

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

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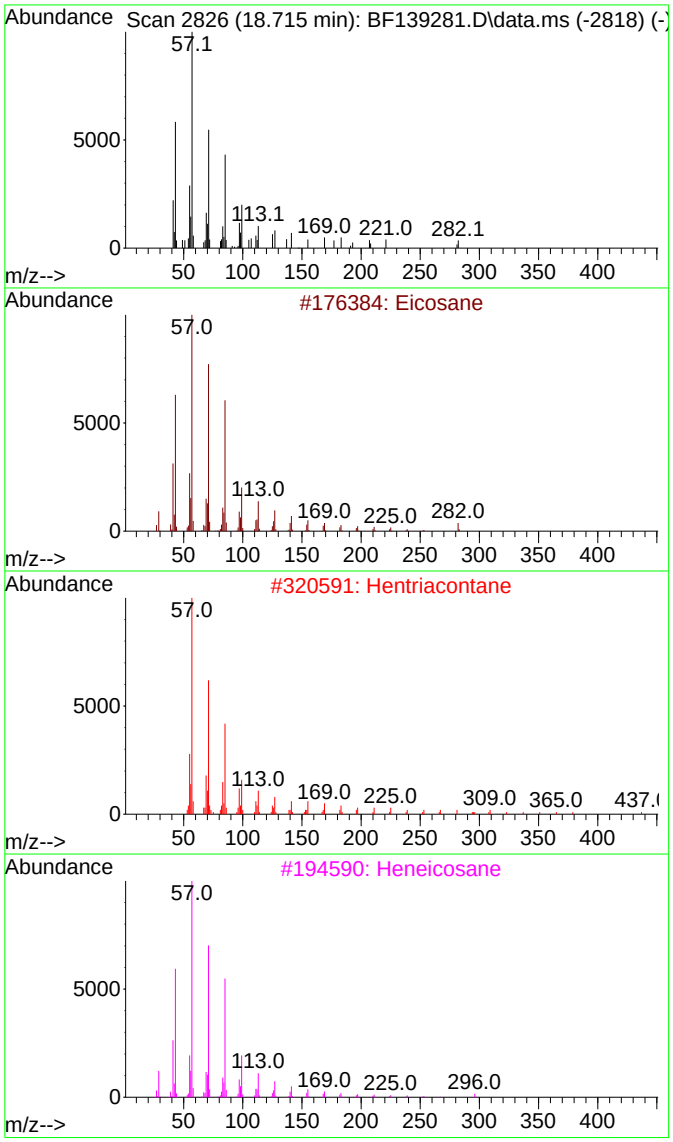
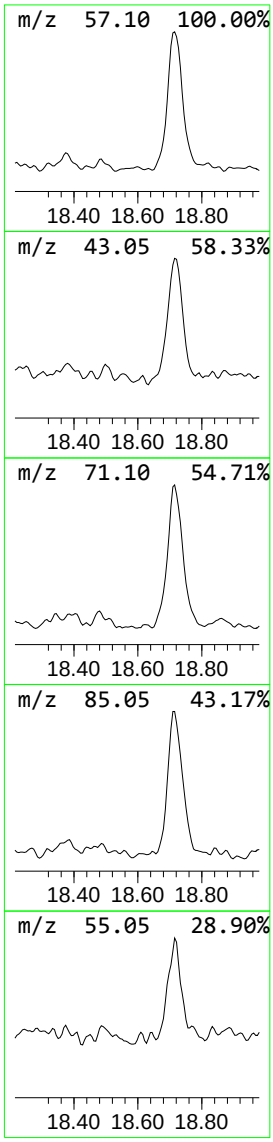
Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.715	2.01 ng	75362	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Hentriacontane	437	C31H64	000630-04-6	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Pentacosane	352	C25H52	000629-99-2	87





Tentatively Identified Compound (LSC) summary

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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB163214BL

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...	2.246	2.9	ng	145160	1	6.887	1017280	20.0
2-Pentanone, 4-...	5.134	6.8	ng	344750	1	6.887	1017280	20.0
Octacosane, 2-m...	16.009	3.6	ng	133796	6	15.527	749466	20.0
Tetratetracontane	16.527	4.1	ng	152174	6	15.527	749466	20.0
Hentriacontane	17.139	3.1	ng	117391	6	15.527	749466	20.0
Heneicosane	17.857	3.1	ng	116255	6	15.527	749466	20.0
Eicosane	18.715	2.0	ng	75362	6	15.527	749466	20.0