LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125148.D
Acq On : 23 Aug 2021 10:17
Operator : JU/CG
Sample : PB138531BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB138531BL

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-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125148.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	24	34	39	rVB	104712	147540	2.89%	0.438%
2	5.175	518	525	533	rVB	133284	187431	3.67%	0.557%
3	5.551	583	589	592	rBV	4676750	4776269	93.44%	14.182%
4	6.545	752	758	761	rBV	4068471	4714583	92.23%	13.999%
5	6.922	818	822	825	rBV	1260910	999511	19.55%	2.968%
6	7.486	912	918	921	rBV	3109726	3100508	60.66%	9.206%
7	8.204	1036	1040	1044	rBV	1531727	1287969	25.20%	3.824%
8	9.280	1218	1223	1226	rBV	5285057	5111495	100.00%	15.178%
9	9.963	1334	1339	1342	rBV	1718540	1388004	27.15%	4.121%
10	10.751	1468	1473	1476	rBV	3529695	3238424	63.36%	9.616%
11	11.451	1588	1592	1595	rBV	1667277	1364225	26.69%	4.051%
12	13.039	1857	1862	1865	rBV	5309266	4925918	96.37%	14.627%
13	14.092	2037	2041	2044	rBV	1151888	1007133	19.70%	2.991%
14	15.221	2230	2233	2240	rVB	54265	67958	1.33%	0.202%
15	15.592	2291	2296	2305	rBV	704476	961717	18.81%	2.856%
16	16.074	2374	2378	2384	rVB	75844	110013	2.15%	0.327%
17	16.598	2463	2467	2475	rVB2	66392	124257	2.43%	0.369%
18	17.221	2569	2573	2579	rBV2	42878	75915	1.49%	0.225%
19	17.956	2694	2698	2707	rVB5	37738	88760	1.74%	0.264%

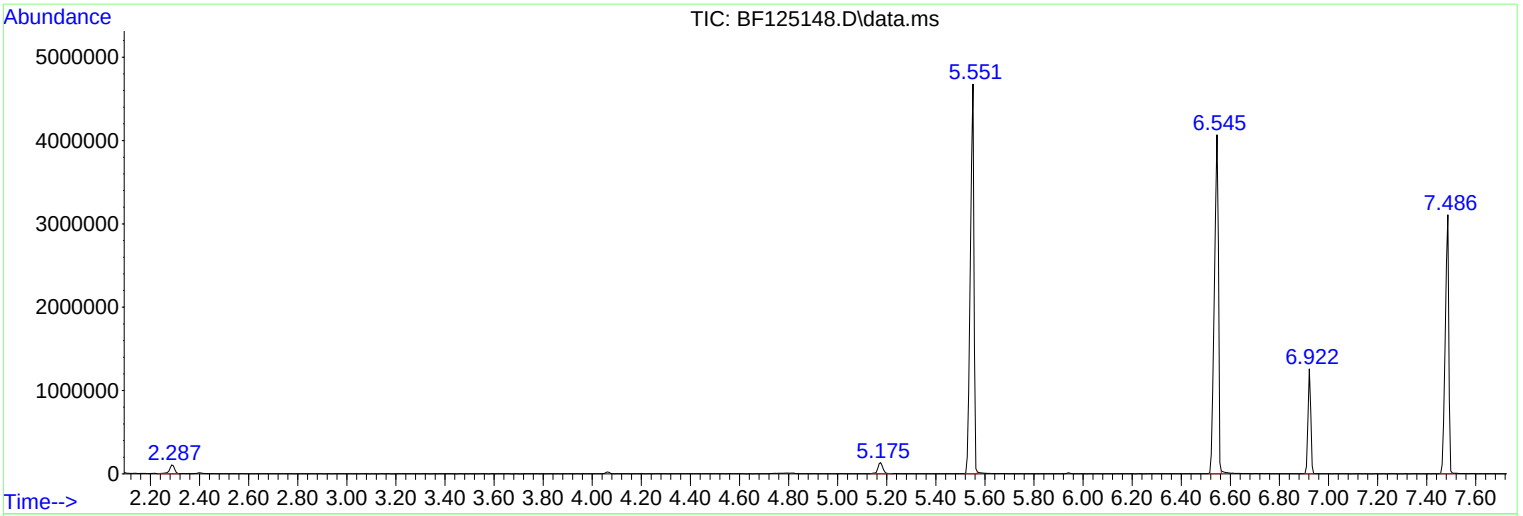
Sum of corrected areas: 33677630

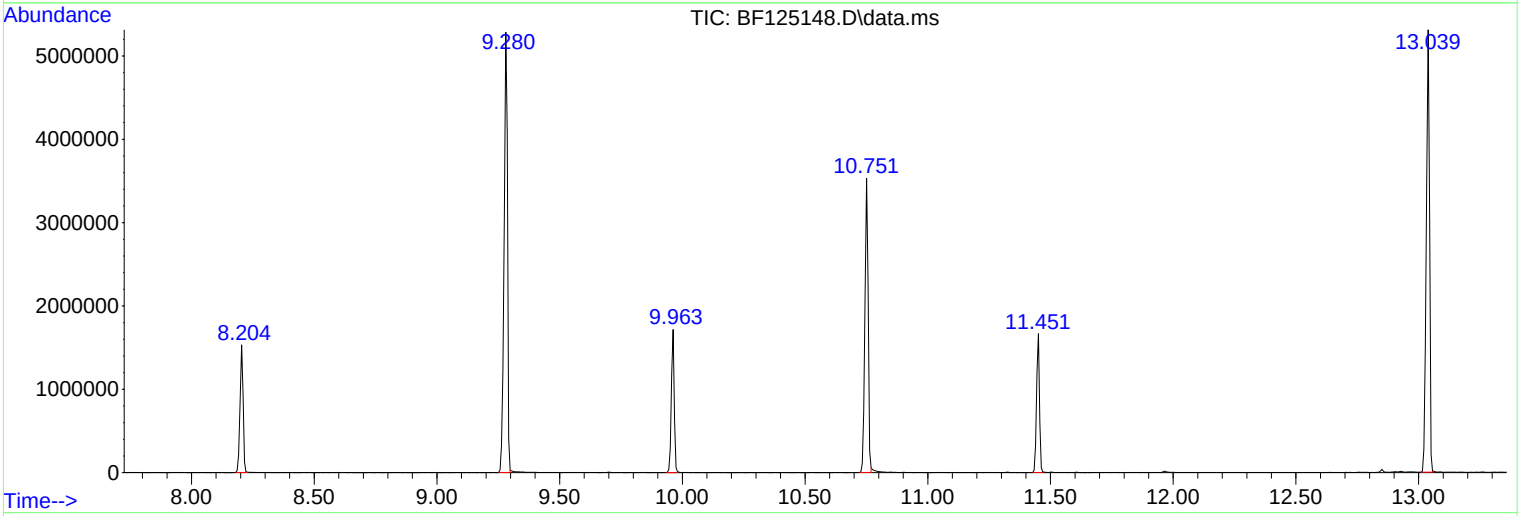
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125148.D
Acq On : 23 Aug 2021 10:17
Operator : JU/CG
Sample : PB138531BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

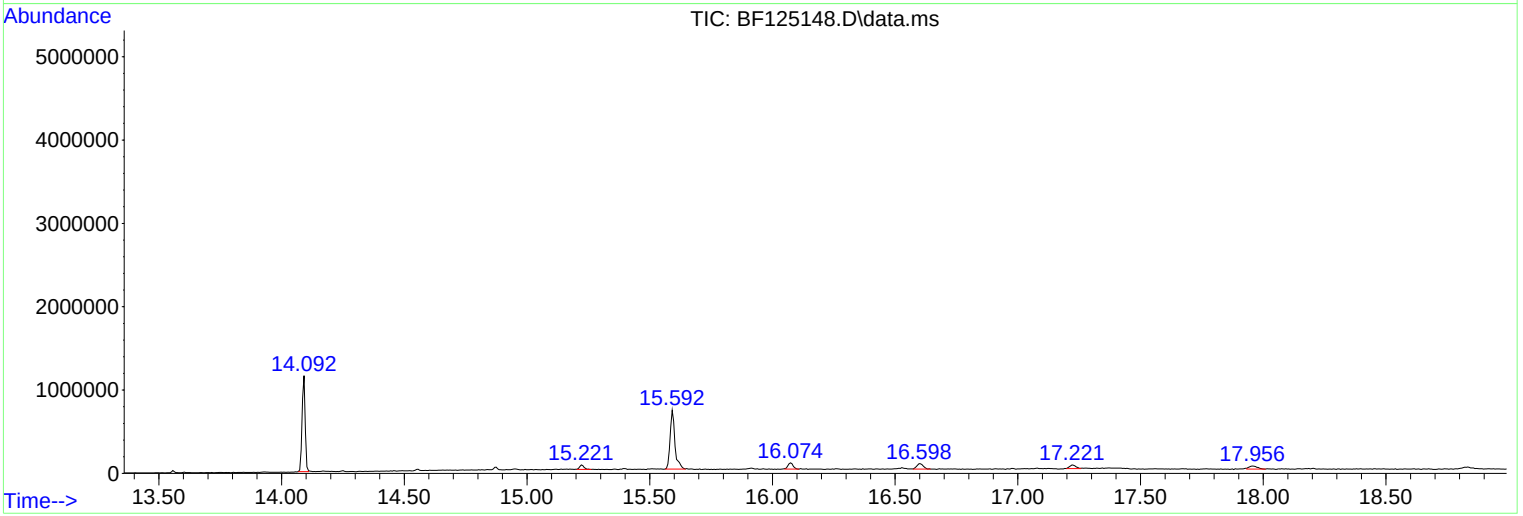
Instrument :
BNA_F
ClientSampleId :
PB138531BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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\BF082321\
Data File : BF125148.D
Acq On : 23 Aug 2021 10:17
Operator : JU/CG
Sample : PB138531BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB138531BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

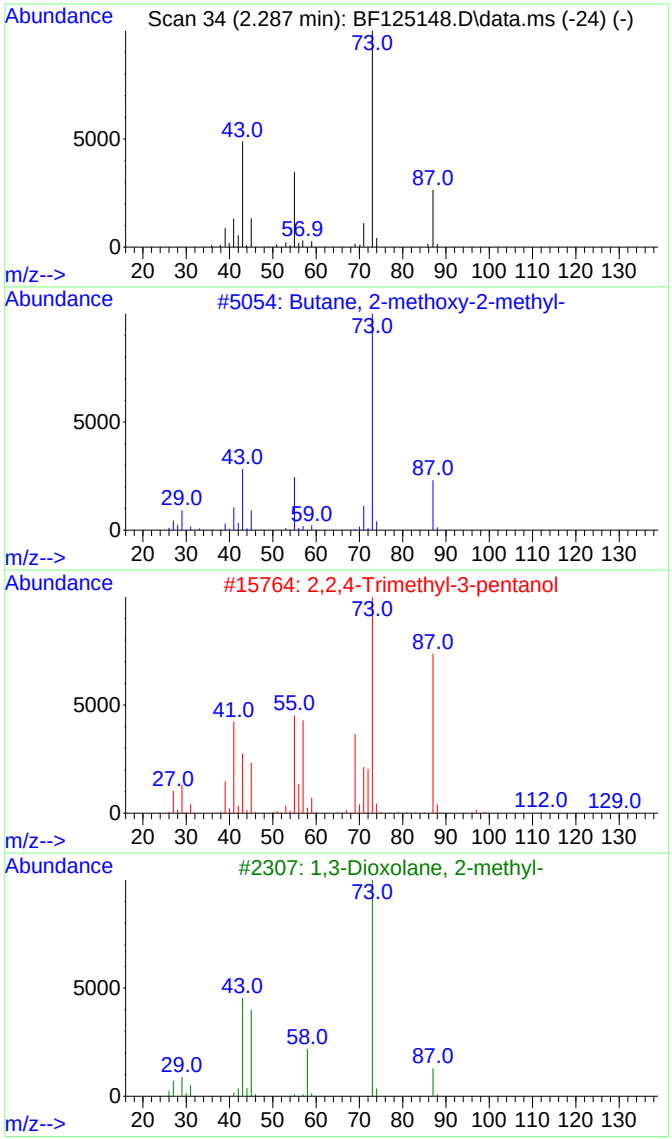
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

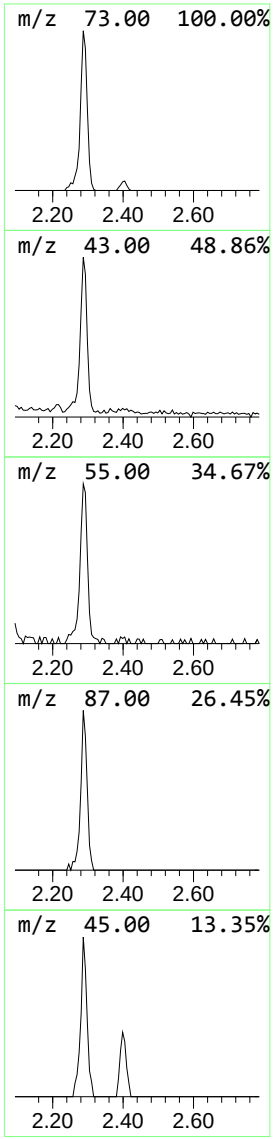
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	2.95 ng	147540	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125148.D
Acq On : 23 Aug 2021 10:17
Operator : JU/CG
Sample : PB138531BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB138531BL

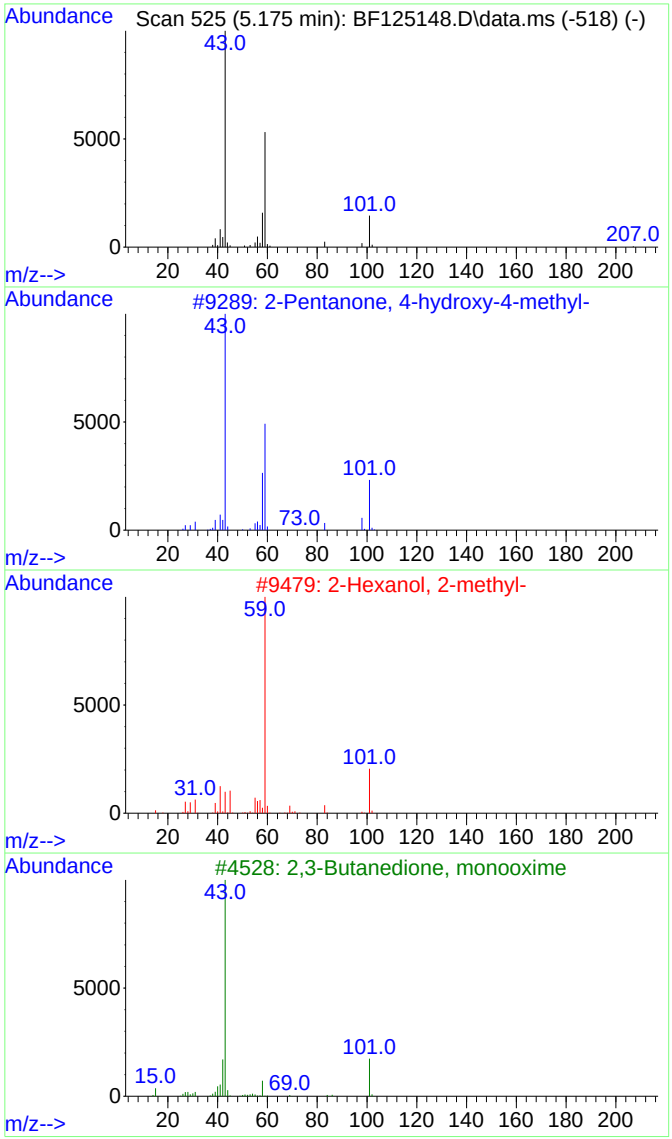
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

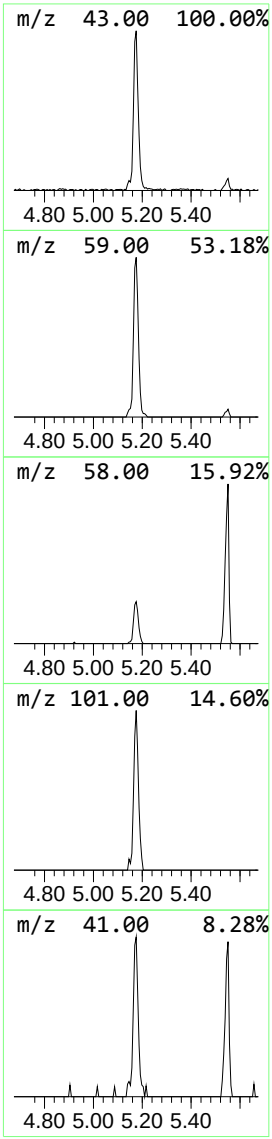
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.175	3.75 ng	187431	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125148.D
Acq On : 23 Aug 2021 10:17
Operator : JU/CG
Sample : PB138531BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB138531BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

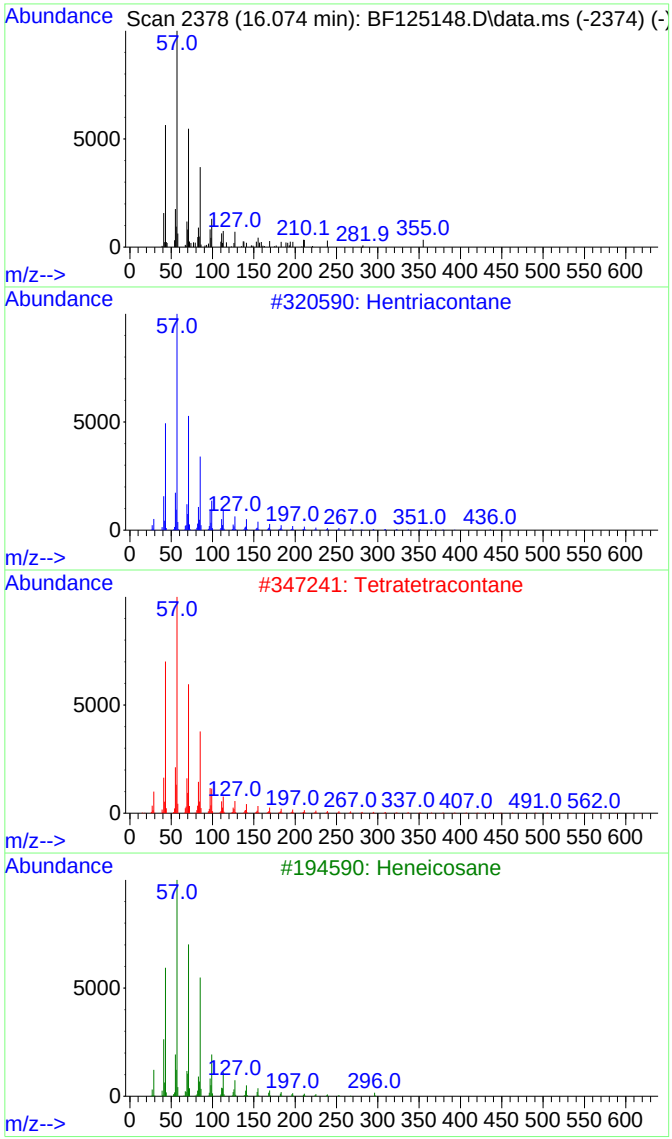
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

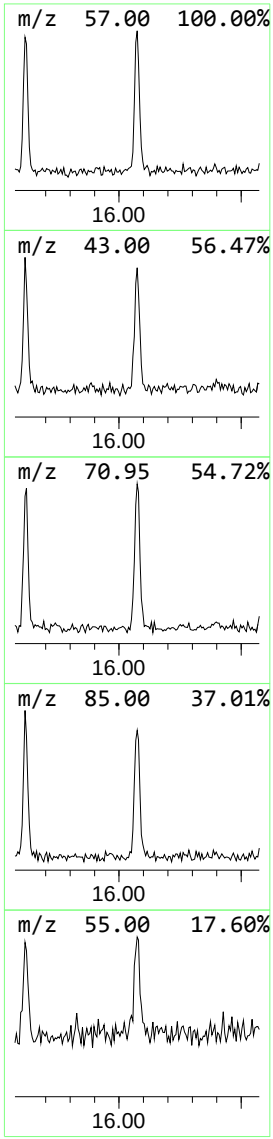
****

Peak Number 3 Hentriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.074	2.29 ng	110013	Perylene-d12	15.592

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	87
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Octadecane	254	C18H38	000593-45-3	86
5	Docosane	310	C22H46	000629-97-0	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125148.D
Acq On : 23 Aug 2021 10:17
Operator : JU/CG
Sample : PB138531BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB138531BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

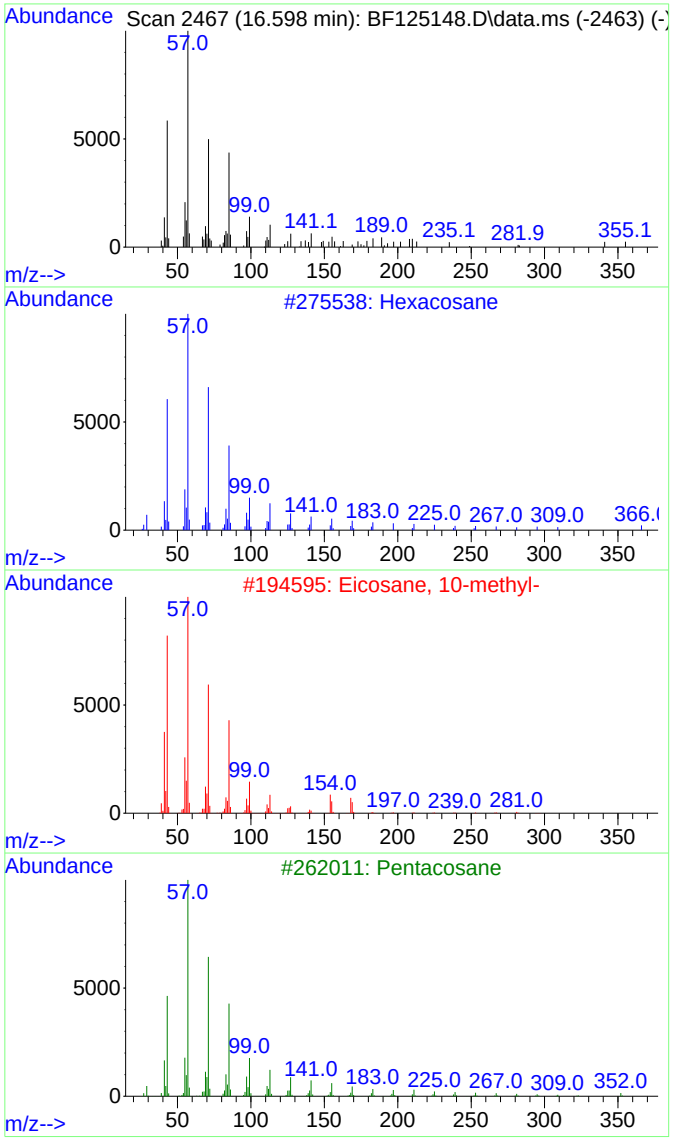
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

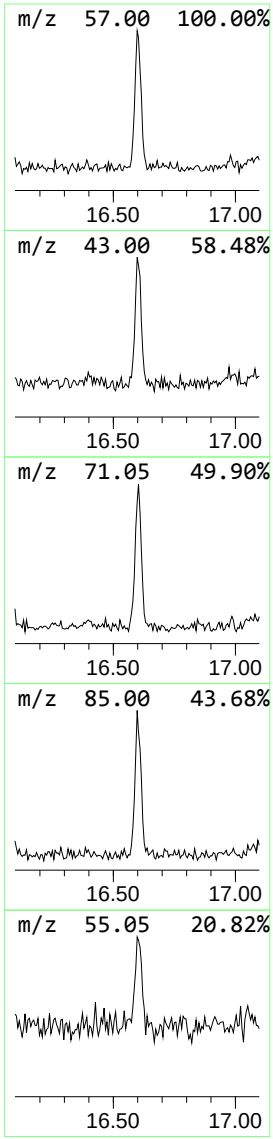
****

Peak Number 4 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.598	2.58 ng	124257	Perylene-d12	15.592

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	83
3	Pentacosane	352	C25H52	000629-99-2	83
4	Heneicosane	296	C21H44	000629-94-7	83
5	Triacontane	422	C30H62	000638-68-6	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125148.D
Acq On : 23 Aug 2021 10:17
Operator : JU/CG
Sample : PB138531BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB138531BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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	3.0	ng	147540	1	6.922	999511	20.0
2-Pentanone, 4-...	5.175	3.8	ng	187431	1	6.922	999511	20.0
Hentriacontane	16.074	2.3	ng	110013	6	15.592	961717	20.0
Hexacosane	16.598	2.6	ng	124257	6	15.592	961717	20.0