LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011822\
Data File : BF126603.D
Acq On : 18 Jan 2022 14:55
Operator : CG/JU
Sample : PB141938BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141938BL

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-BF011822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126603.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.369	38	48	54	rVB	112248	163313	3.14%	0.502%
2	5.593	590	596	599	rBV	3336032	3927251	75.60%	12.081%
3	6.575	757	763	766	rBV	3252509	4118537	79.28%	12.670%
4	6.963	825	829	832	rVB	970739	788720	15.18%	2.426%
5	7.522	919	924	927	rBV	2346590	2684777	51.68%	8.259%
6	8.245	1042	1047	1050	rBV	1122710	1086074	20.91%	3.341%
7	9.322	1224	1230	1233	rBV	3961245	4533037	87.26%	13.945%
8	10.004	1340	1346	1350	rBV	1391668	1305397	25.13%	4.016%
9	10.798	1474	1481	1484	rBV	2818824	2992460	57.60%	9.206%
10	11.498	1594	1600	1603	rBV	1581655	1389017	26.74%	4.273%
11	13.098	1864	1872	1875	rBV	4693808	5195047	100.00%	15.982%
12	14.174	2048	2055	2058	rBV	1418232	1270069	24.45%	3.907%
13	14.674	2138	2140	2147	rVB	55662	61090	1.18%	0.188%
14	15.010	2193	2197	2201	rVB	113450	110909	2.13%	0.341%
15	15.380	2255	2260	2266	rVB	165262	193737	3.73%	0.596%
16	15.745	2316	2322	2326	rBV	920732	1137312	21.89%	3.499%
17	15.792	2326	2330	2336	rVB	236786	300057	5.78%	0.923%
18	16.268	2405	2411	2419	rBV	192973	309253	5.95%	0.951%
19	16.821	2497	2505	2514	rBV	165496	304216	5.86%	0.936%
20	17.474	2609	2616	2625	rBV	97971	211607	4.07%	0.651%
21	17.939	2678	2695	2708	rBV4	53105	239955	4.62%	0.738%
22	18.245	2738	2747	2757	rBV2	69046	184785	3.56%	0.568%

Sum of corrected areas: 32506620

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011822\
Data File : BF126603.D
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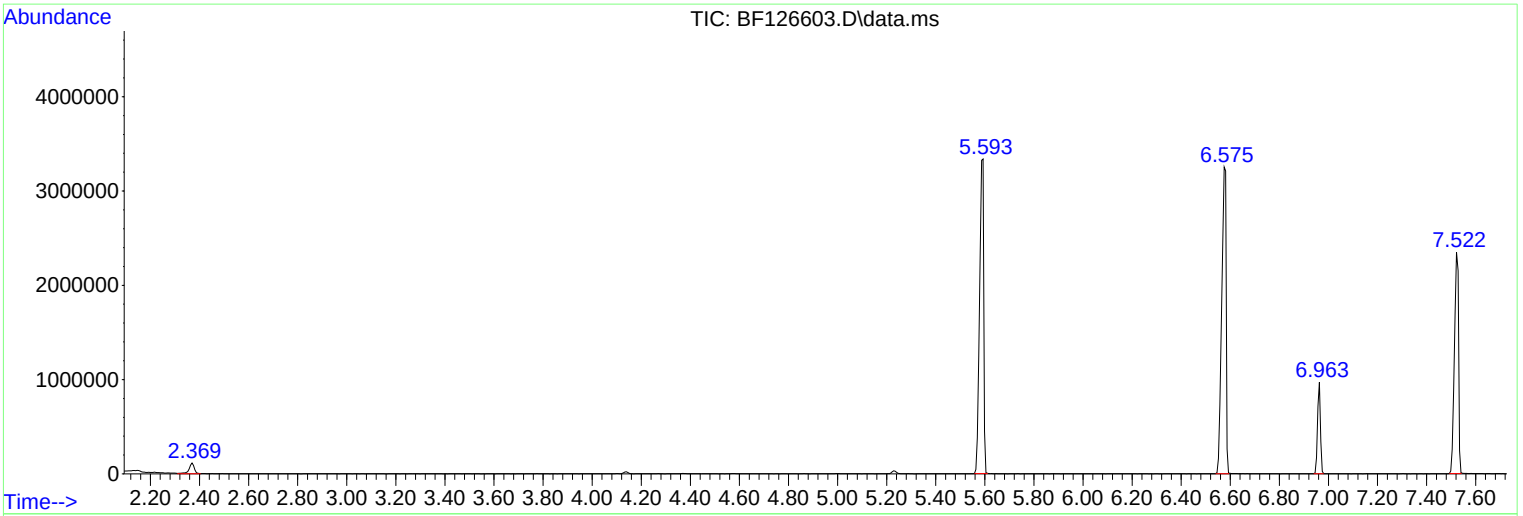
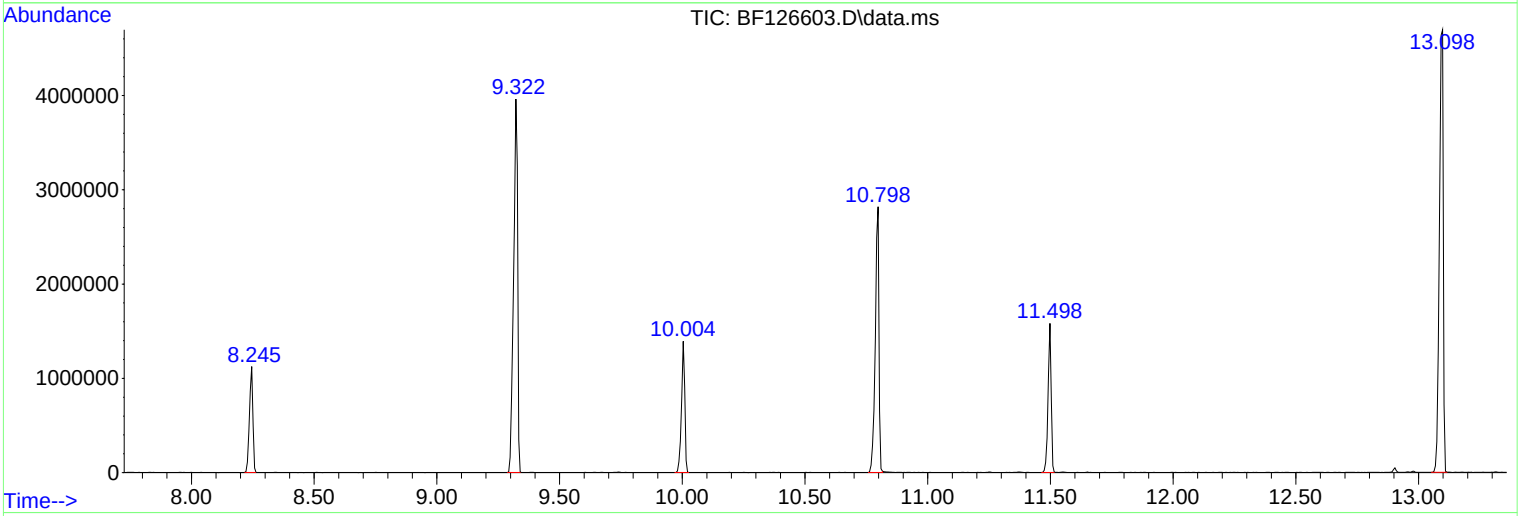
Operator : CG/JU
Sample : PB141938BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

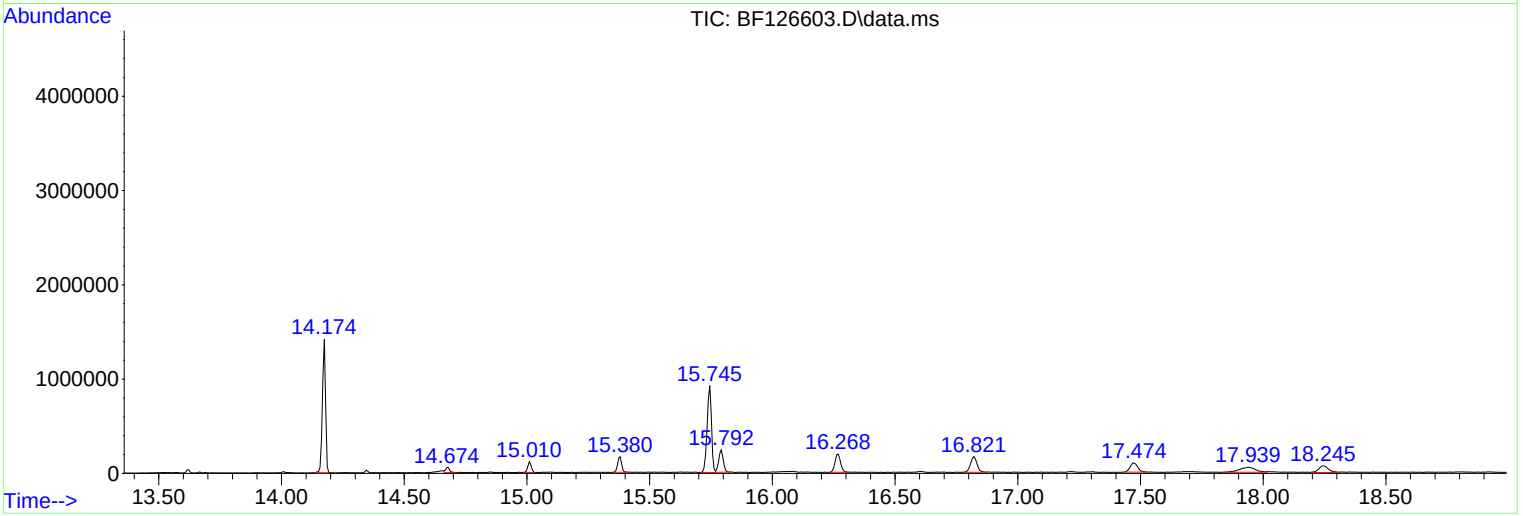
Instrument :
BNA_F
ClientSampleId :
PB141938BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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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Data File : BF126603.D
Acq On : 18 Jan 2022 14:55
Operator : CG/JU
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

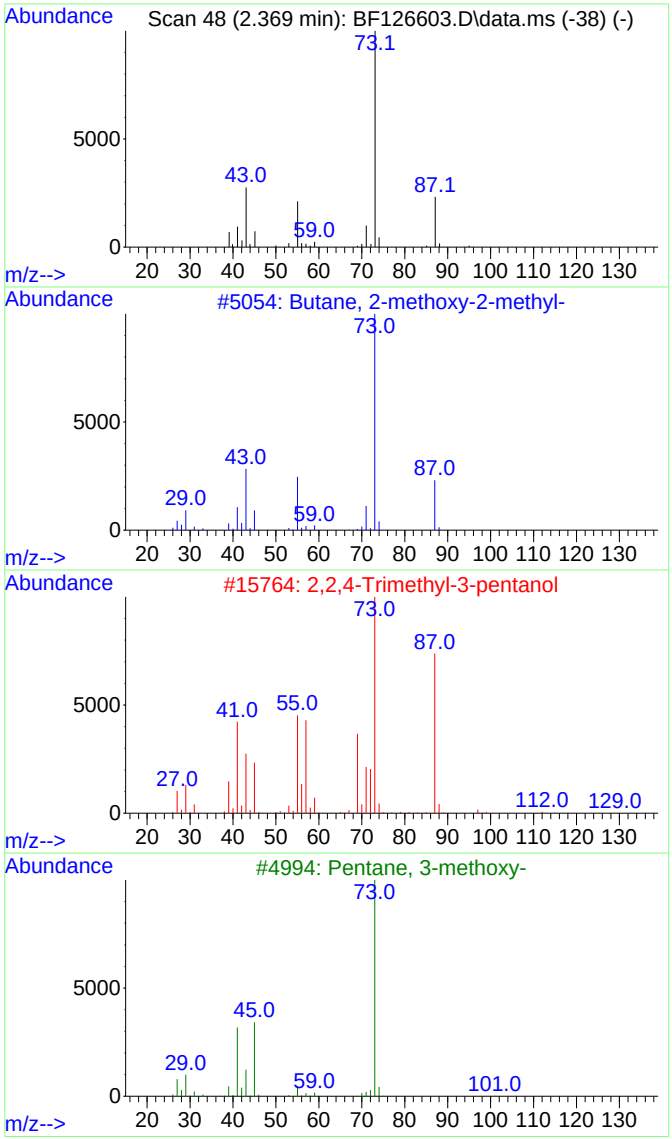
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

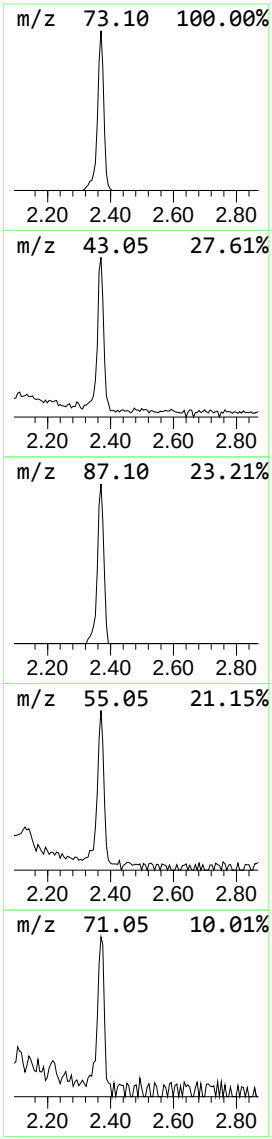
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.369	4.14 ng	163313	1,4-Dichlorobenzene-d4	6.963

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	43
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Data File : BF126603.D
Acq On : 18 Jan 2022 14:55
Operator : CG/JU
Sample : PB141938BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141938BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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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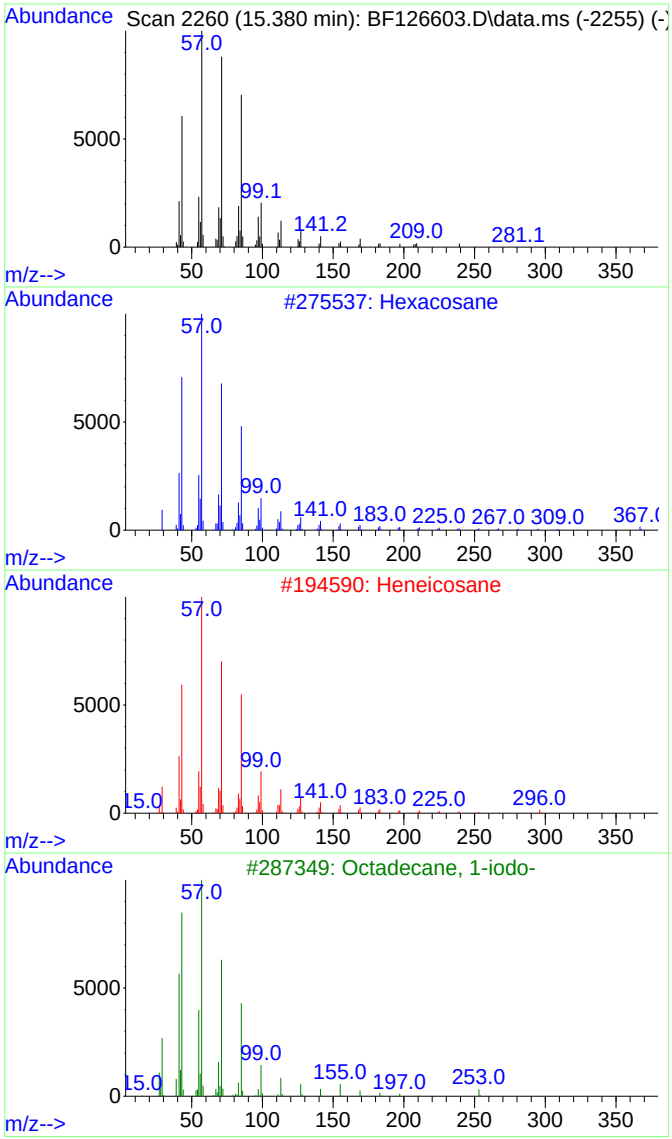
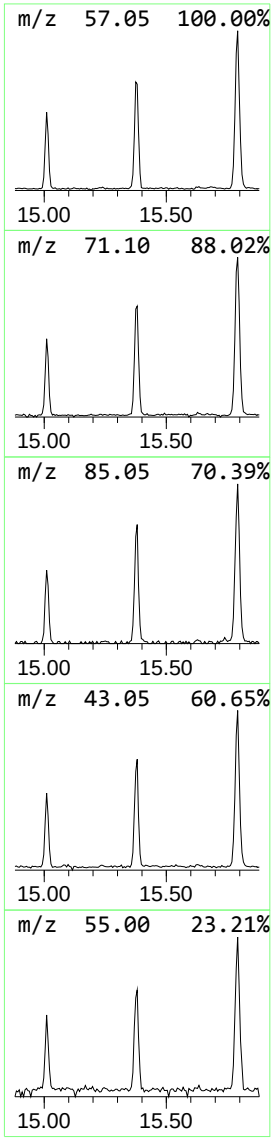
Peak Number 2 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	3.41 ng	193737	Perylene-d12	15.745

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	90
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1010115-66-1	86
5	10-Methylnonadecane	282	C20H42	056862-62-5	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011822\
Data File : BF126603.D
Acq On : 18 Jan 2022 14:55
Operator : CG/JU
Sample : PB141938BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141938BL

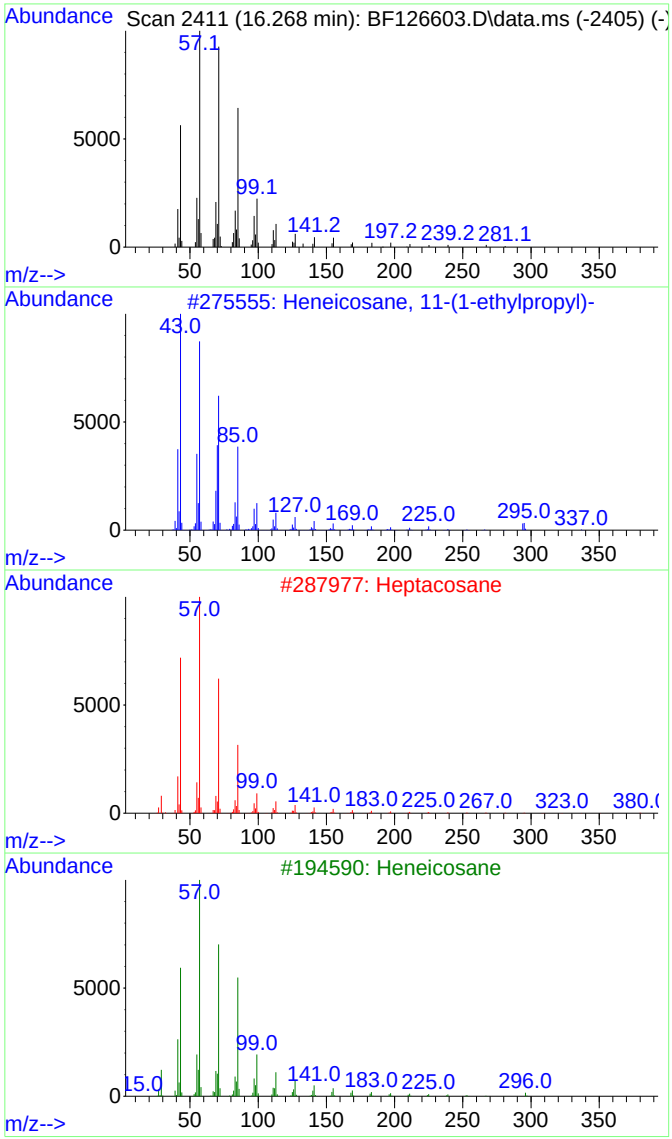
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

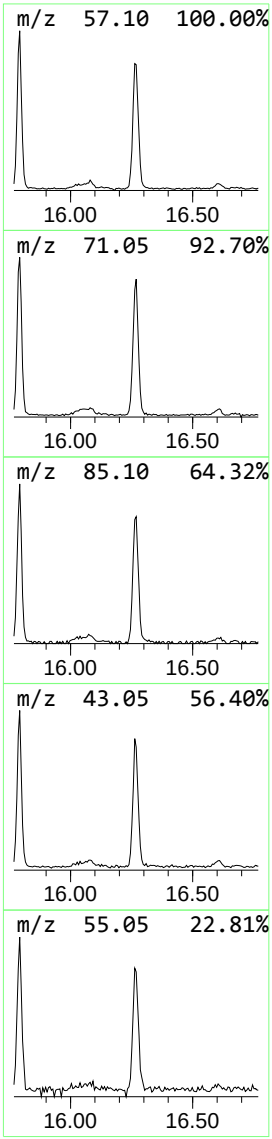
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Heneicosane, 11-(1-ethylpro... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.268	5.44 ng	309253	Perylene-d12	15.745

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
2	Heptacosane	380	C27H56	000593-49-7	83
3	Heneicosane	296	C21H44	000629-94-7	68
4	Hexacosane	366	C26H54	000630-01-3	62
5	Tetratetracontane	619	C44H90	007098-22-8	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011822\
Data File : BF126603.D
Acq On : 18 Jan 2022 14:55
Operator : CG/JU
Sample : PB141938BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141938BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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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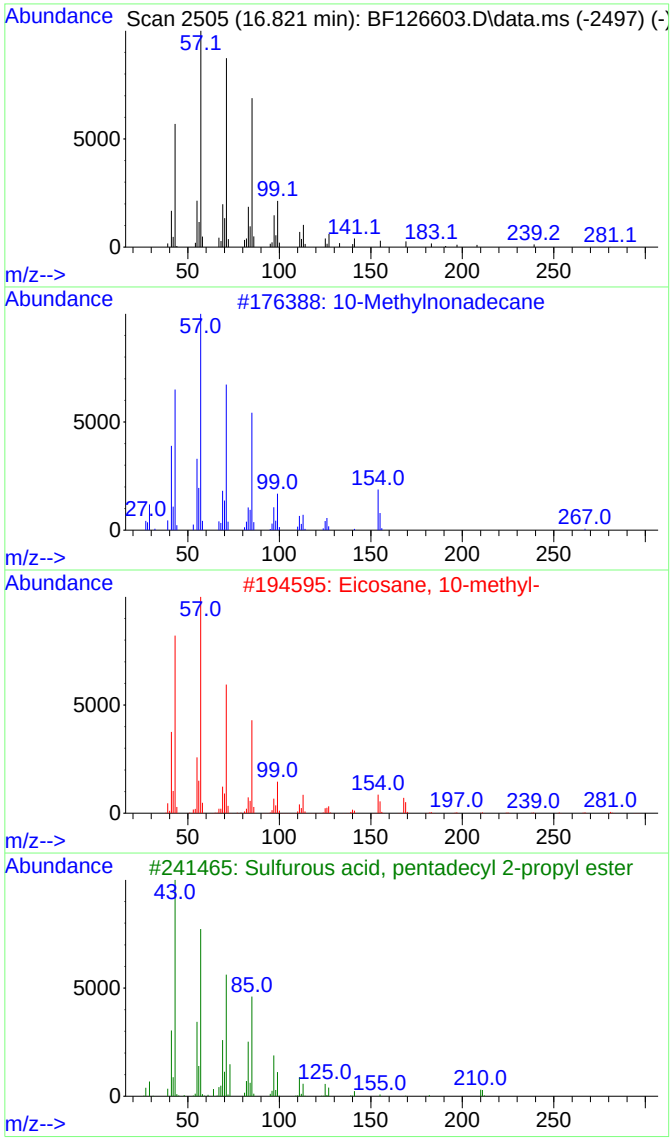
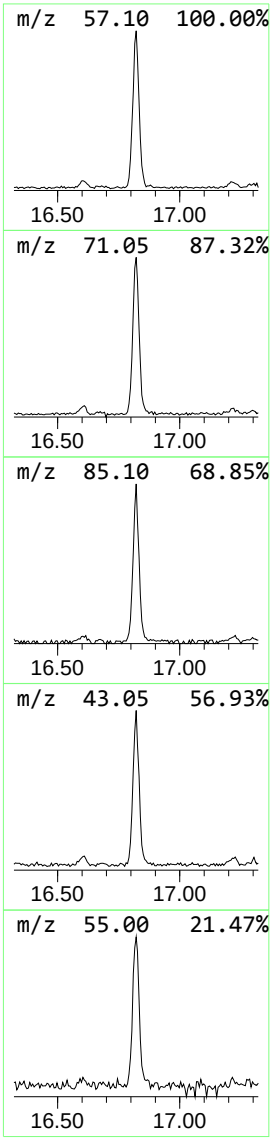
Peak Number 4 10-Methylnonadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.821	5.35 ng	304216	Perylene-d12	15.745

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Methylnonadecane	282	C20H42	056862-62-5	90
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	86
3	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	72
4	Heneicosane	296	C21H44	000629-94-7	64
5	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011822\
Data File : BF126603.D
Acq On : 18 Jan 2022 14:55
Operator : CG/JU
Sample : PB141938BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141938BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

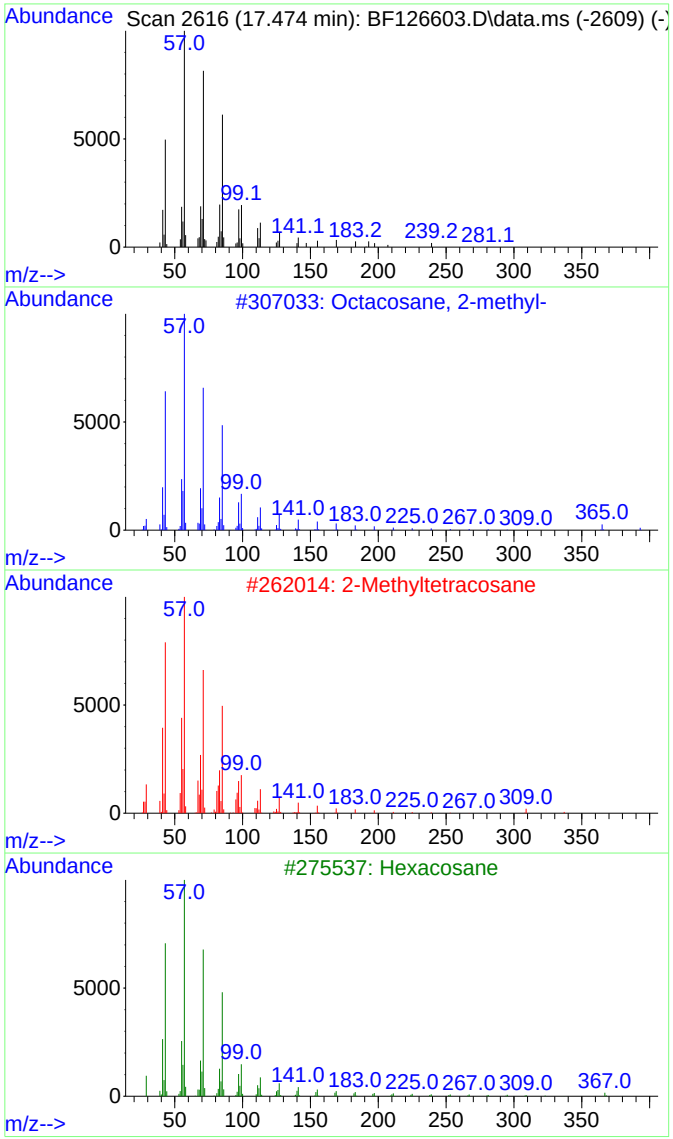
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

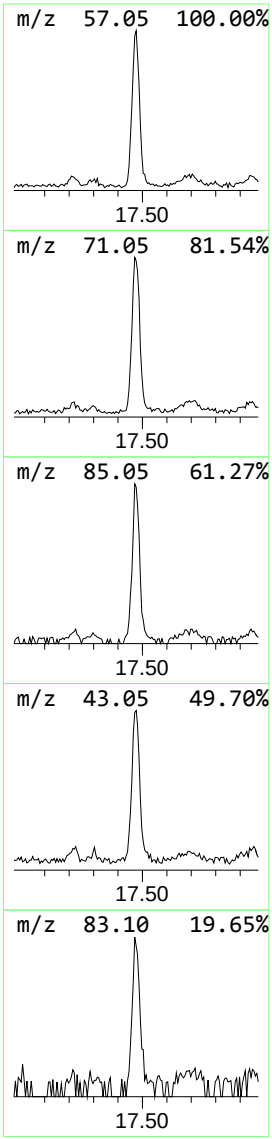
****

Peak Number 5 Octacosane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.474	3.72 ng	211607	Perylene-d12	15.745

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
2	2-Methyltetracosane	352	C25H52	001560-78-7	90
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Heptadecane	240	C17H36	000629-78-7	83





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Data File : BF126603.D
Acq On : 18 Jan 2022 14:55
Operator : CG/JU
Sample : PB141938BL
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB141938BL

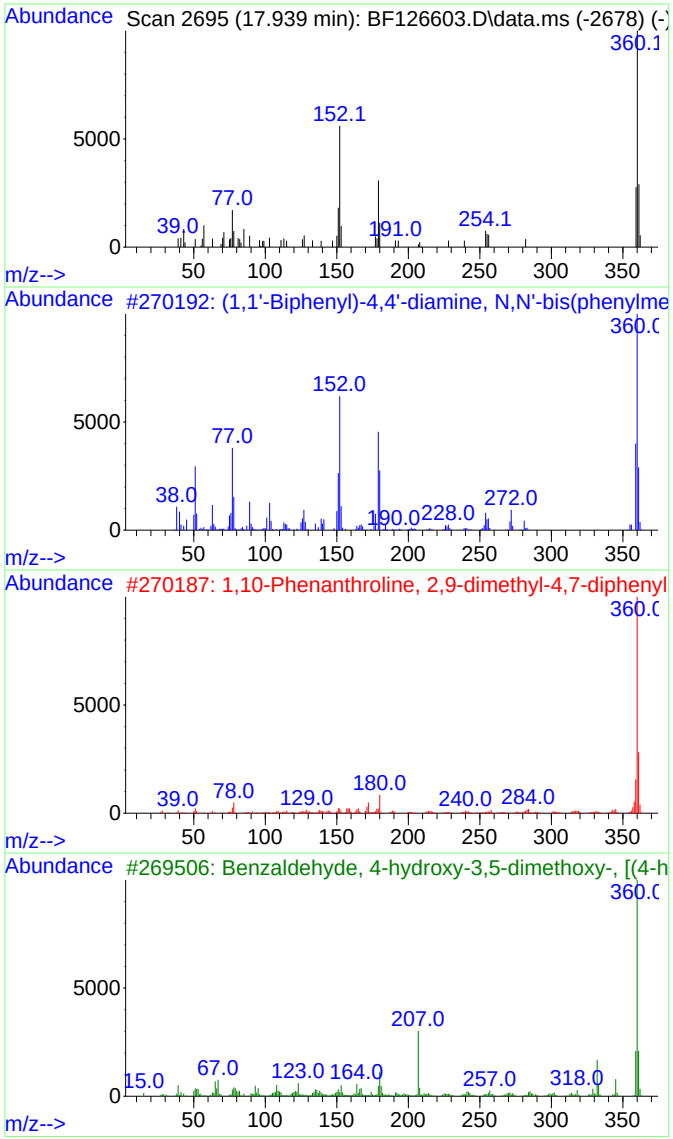
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

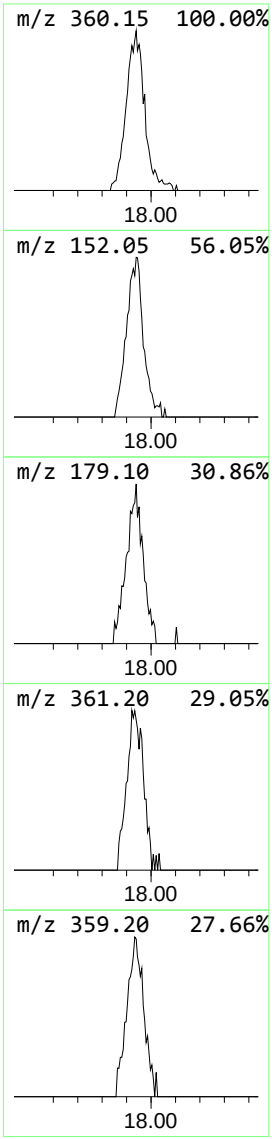
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.939	4.22 ng	239955	Perylene-d12	15.745

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	90
2	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	47
3	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	47
4	N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	43
5	Ethene, 1-(anthracen-9-yl)-2-(4-...	360	C27H20O	1000163-55-1	43





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Sample : PB141938BL
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BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

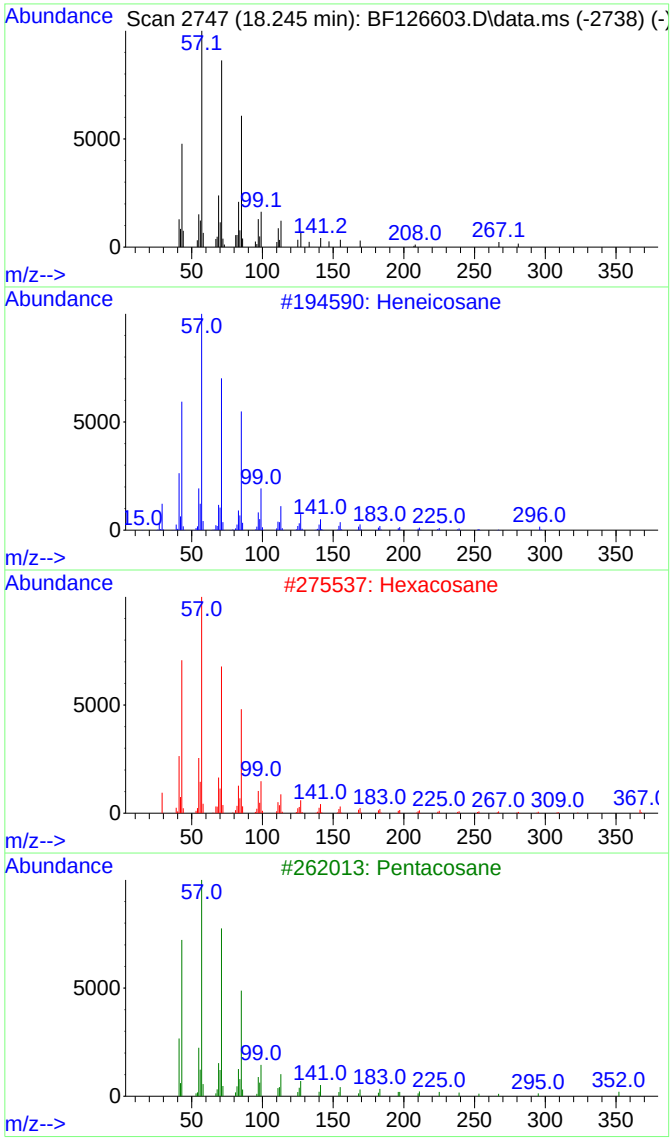
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

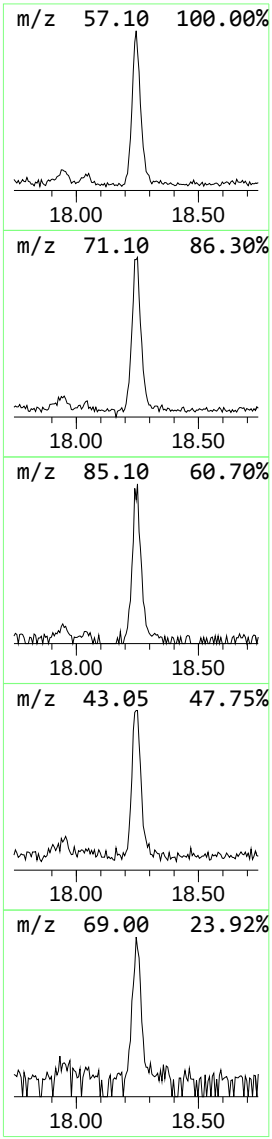
****

Peak Number 7 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.245	3.25 ng	184785	Perylene-d12	15.745

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Hexacosane	366	C26H54	000630-01-3	87
3	Pentacosane	352	C25H52	000629-99-2	86
4	Nonadecane	268	C19H40	000629-92-5	80
5	Tetracosane	338	C24H50	000646-31-1	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011822\
Data File : BF126603.D
Acq On : 18 Jan 2022 14:55
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Sample : PB141938BL
Misc :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011822.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...	2.369	4.1	ng	163313	1	6.963	788720	20.0
Hexacosane	15.380	3.4	ng	193737	6	15.745	1137310	20.0
Heneicosane, 11...	16.268	5.4	ng	309253	6	15.745	1137310	20.0
10-Methylnonade...	16.821	5.3	ng	304216	6	15.745	1137310	20.0
Octacosane, 2-m...	17.474	3.7	ng	211607	6	15.745	1137310	20.0
(1,1'-Biphenyl)...	17.939	4.2	ng	239955	6	15.745	1137310	20.0
Heneicosane	18.245	3.3	ng	184785	6	15.745	1137310	20.0