LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125303.D
Acq On : 1 Sep 2021 13:24
Operator : JU/CG
Sample : M3612-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-1

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: BF125303.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.163	8	13	27	rVB	928929	1225009	28.32%	3.632%
2	5.522	580	584	588	rBV	3148586	3007923	69.53%	8.918%
3	6.534	751	756	759	rBV	3241928	3019145	69.78%	8.952%
4	6.904	815	819	823	rBV	1367107	1073017	24.80%	3.181%
5	7.469	910	915	918	rBV	2283675	1957180	45.24%	5.803%
6	8.092	1017	1021	1034	rBV	246867	459682	10.63%	1.363%
7	8.187	1034	1037	1041	rBV	1636350	1443265	33.36%	4.279%
8	9.263	1216	1220	1223	rBV	4294070	3515089	81.25%	10.422%
9	9.945	1332	1336	1340	rBV	2086207	1719653	39.75%	5.099%
10	10.351	1399	1405	1411	rVB	43367	55687	1.29%	0.165%
11	10.733	1466	1470	1474	rBV	2888465	2532284	58.53%	7.508%
12	11.180	1542	1546	1555	rVB	144748	157101	3.63%	0.466%
13	11.433	1585	1589	1593	rBV	2240983	1885534	43.58%	5.591%
14	11.951	1672	1677	1681	rBV	453406	523438	12.10%	1.552%
15	12.169	1709	1714	1725	rVB	18986	57288	1.32%	0.170%
16	12.527	1772	1775	1777	rVB	97364	84136	1.94%	0.249%
17	12.733	1807	1810	1817	rBV	123727	158317	3.66%	0.469%
18	13.022	1854	1859	1862	rBV	4959706	4326360	100.00%	12.828%
19	13.139	1870	1879	1893	rVB2	177523	547742	12.66%	1.624%
20	13.357	1908	1916	1926	rBV2	56714	160307	3.71%	0.475%
21	13.910	2006	2010	2012	rBV2	53867	68811	1.59%	0.204%
22	13.939	2012	2015	2019	rVV	119919	134854	3.12%	0.400%
23	14.074	2035	2038	2042	rBV	1771492	1656441	38.29%	4.911%
24	14.139	2042	2049	2056	rVB	202694	468374	10.83%	1.389%
25	14.533	2113	2116	2119	rBV	53928	47793	1.10%	0.142%
26	14.833	2161	2167	2174	rBV	229798	466847	10.79%	1.384%
27	15.198	2225	2229	2234	rVB	73479	89618	2.07%	0.266%
28	15.574	2287	2293	2307	rBV2	1131501	1788424	41.34%	5.303%
29	16.039	2366	2372	2383	rVB2	131615	296551	6.85%	0.879%
30	16.509	2445	2452	2458	rBV2	99690	282544	6.53%	0.838%
31	17.568	2625	2632	2643	rVB3	81709	247330	5.72%	0.733%
32	18.586	2796	2805	2819	rVB3	65120	271182	6.27%	0.804%

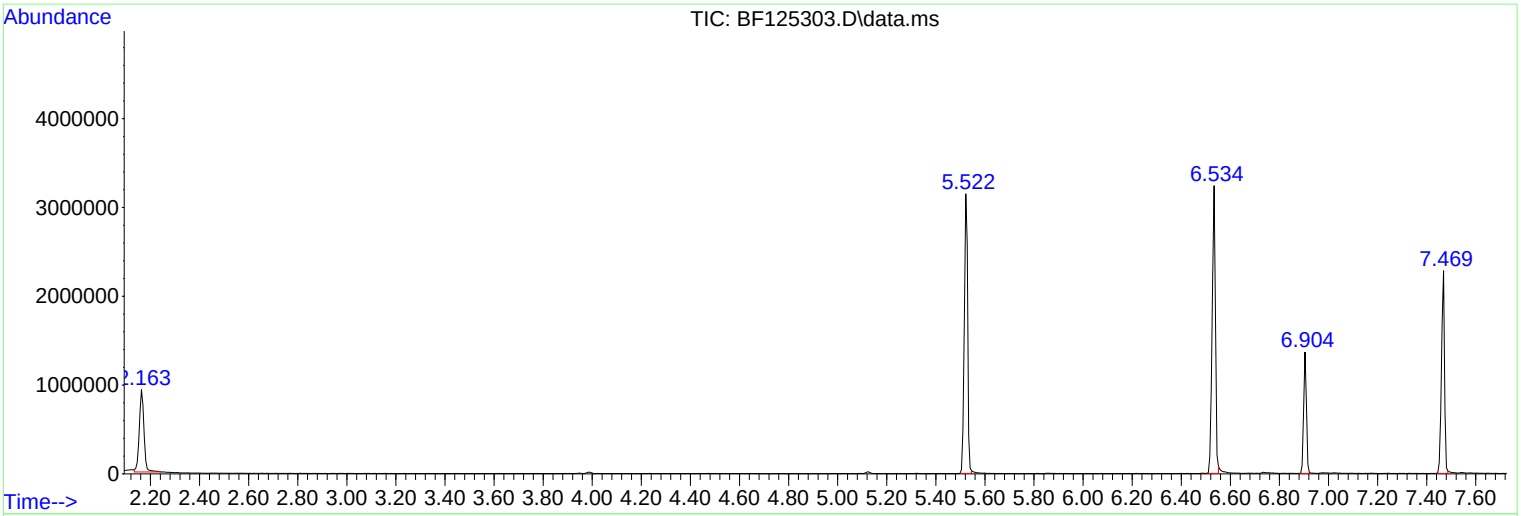
Sum of corrected areas: 33726926

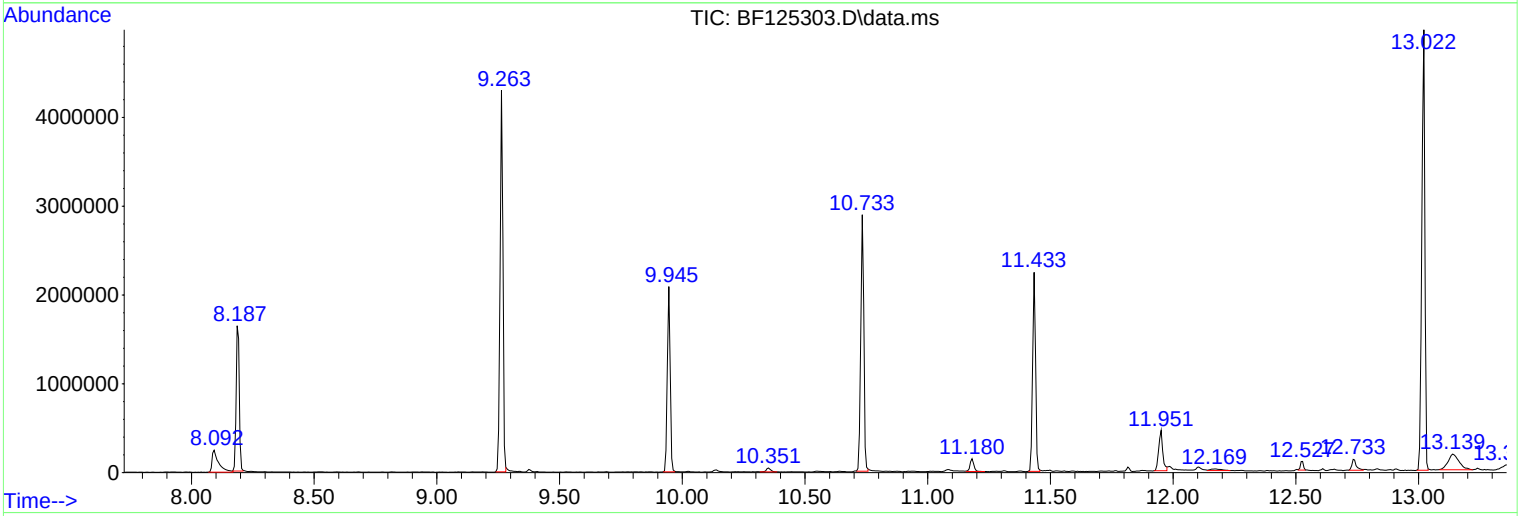
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125303.D
Acq On : 1 Sep 2021 13:24
Operator : JU/CG
Sample : M3612-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

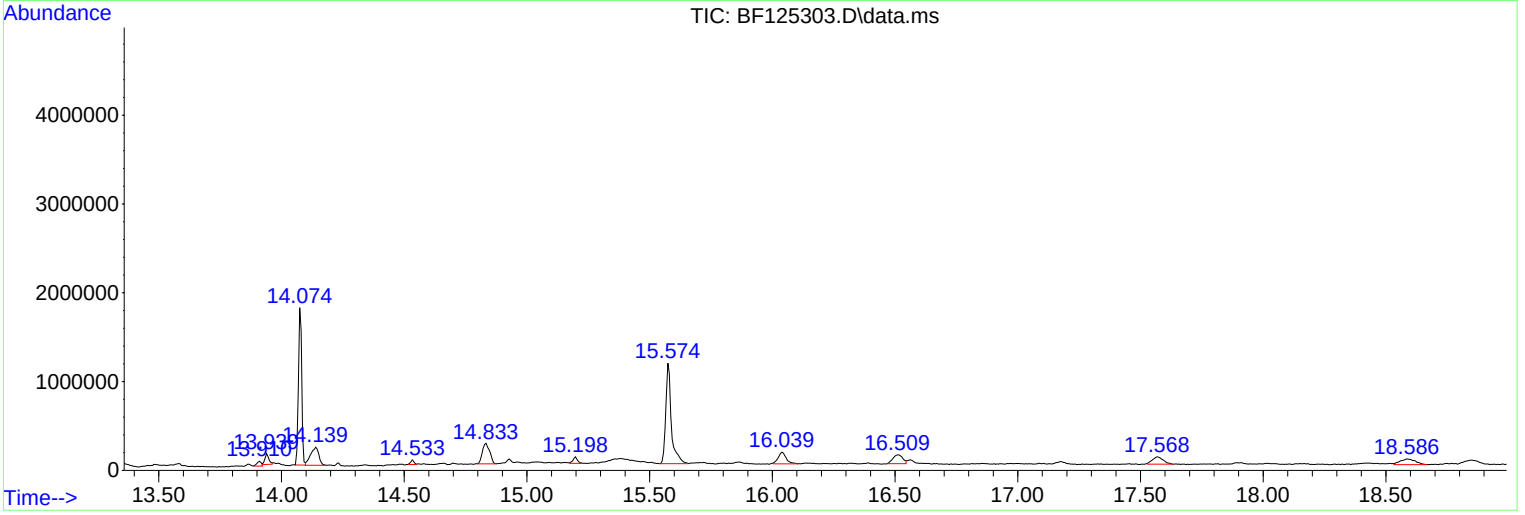
Instrument :
BNA_F
ClientSampleId :
M-1

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\BF090121\
Data File : BF125303.D
Acq On : 1 Sep 2021 13:24
Operator : JU/CG
Sample : M3612-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-1

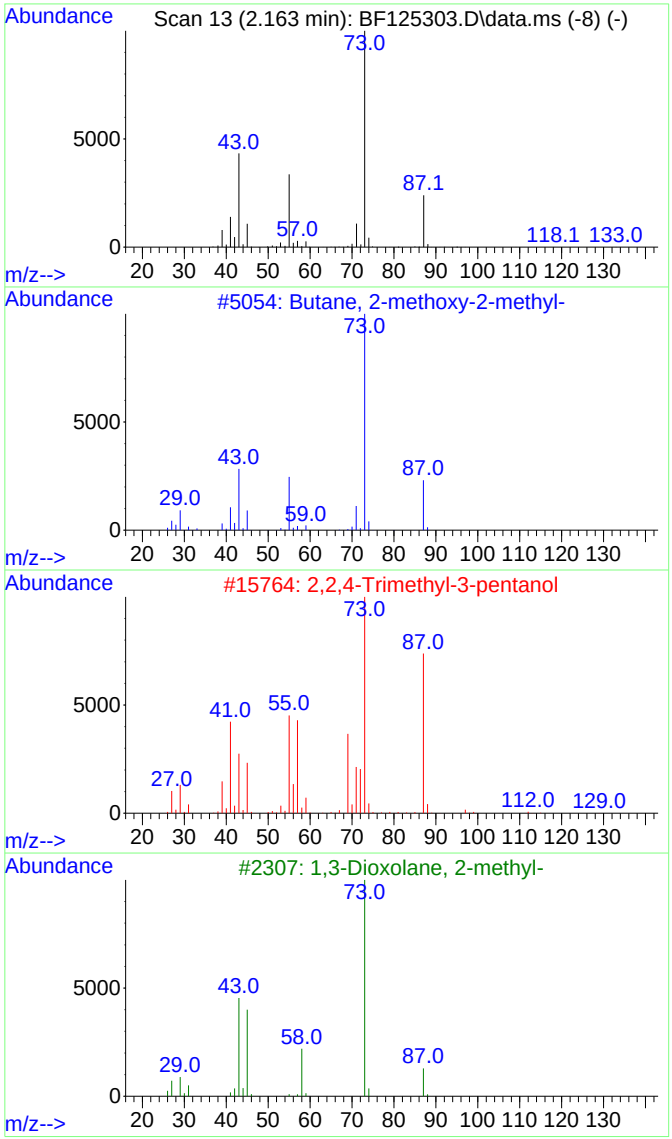
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

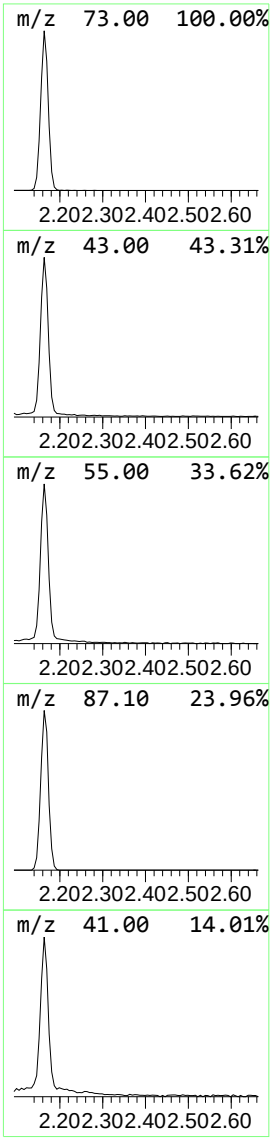
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	22.83 ng	1225010	1,4-Dichlorobenzene-d4	6.904

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	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125303.D
Acq On : 1 Sep 2021 13:24
Operator : JU/CG
Sample : M3612-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-1

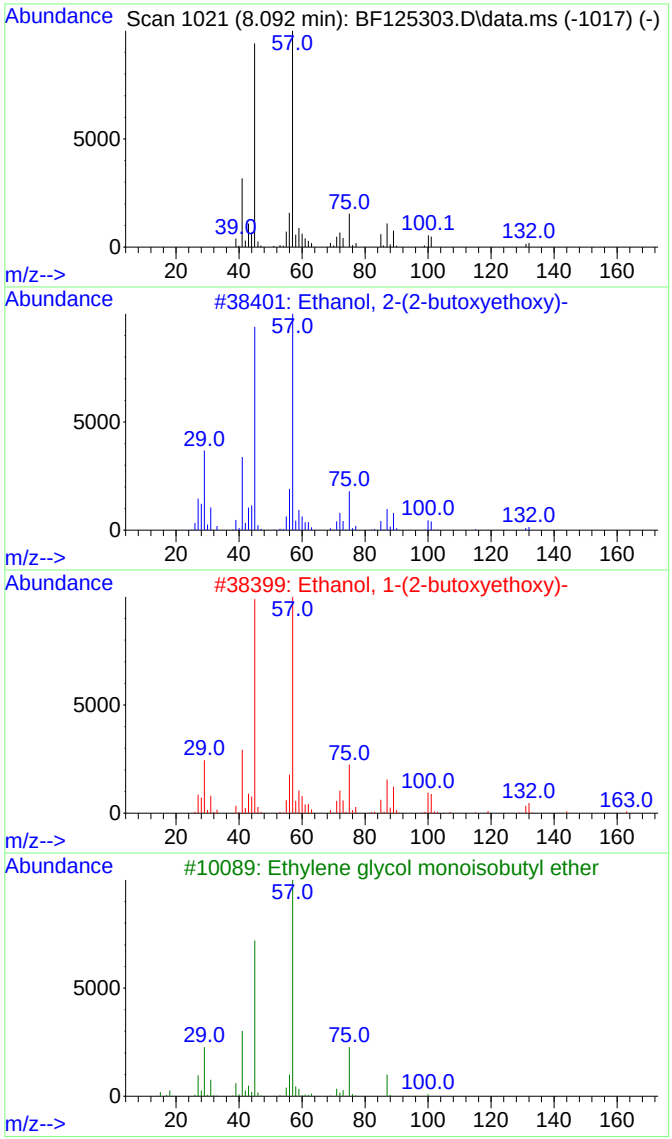
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

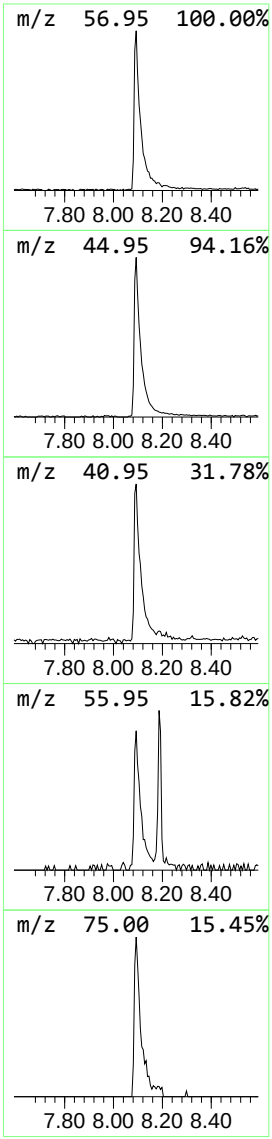
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.092	6.37 ng	459682	Naphthalene-d8	8.187

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125303.D
Acq On : 1 Sep 2021 13:24
Operator : JU/CG
Sample : M3612-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-1

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

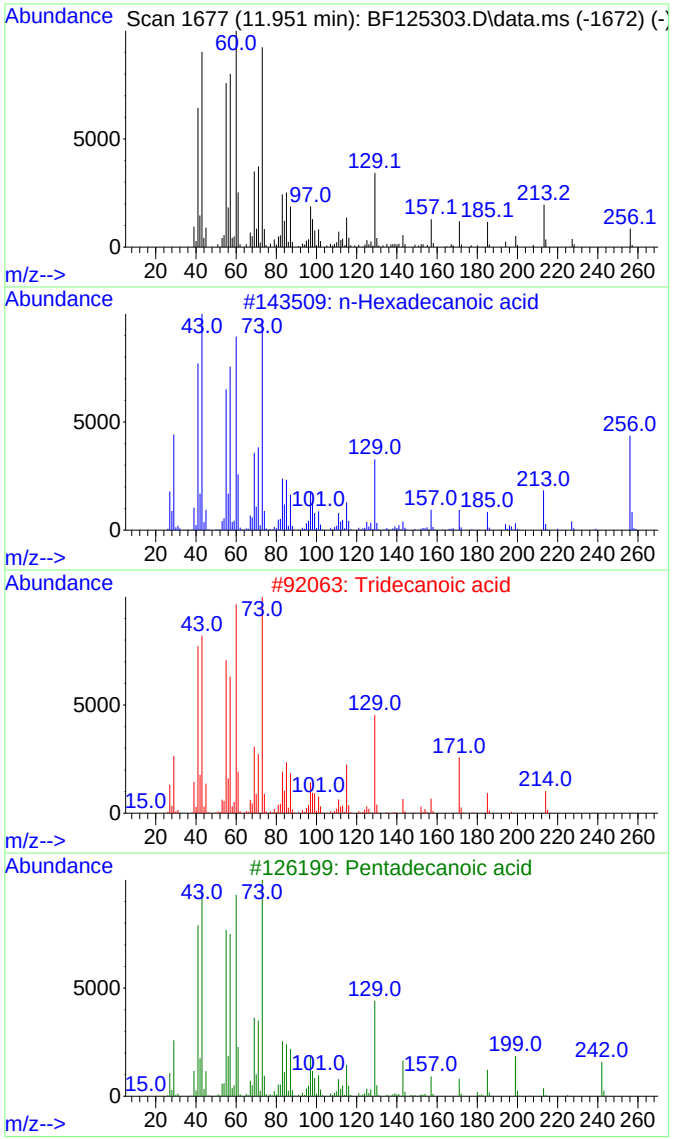
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

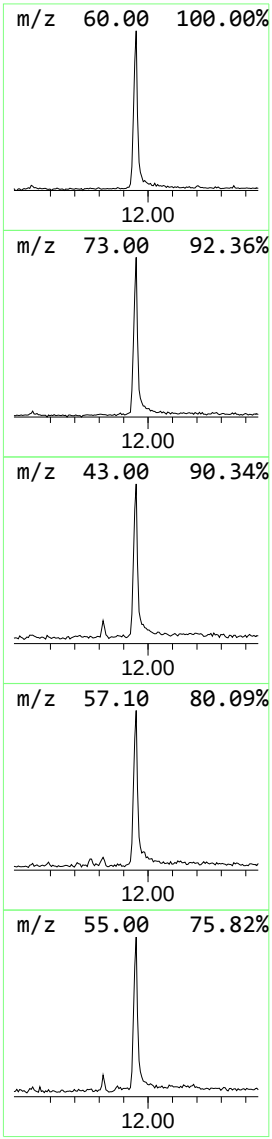
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	5.55 ng	523438	Phenanthrene-d10	11.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Nonanoic acid	158	C9H18O2	000112-05-0	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125303.D
Acq On : 1 Sep 2021 13:24
Operator : JU/CG
Sample : M3612-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-1

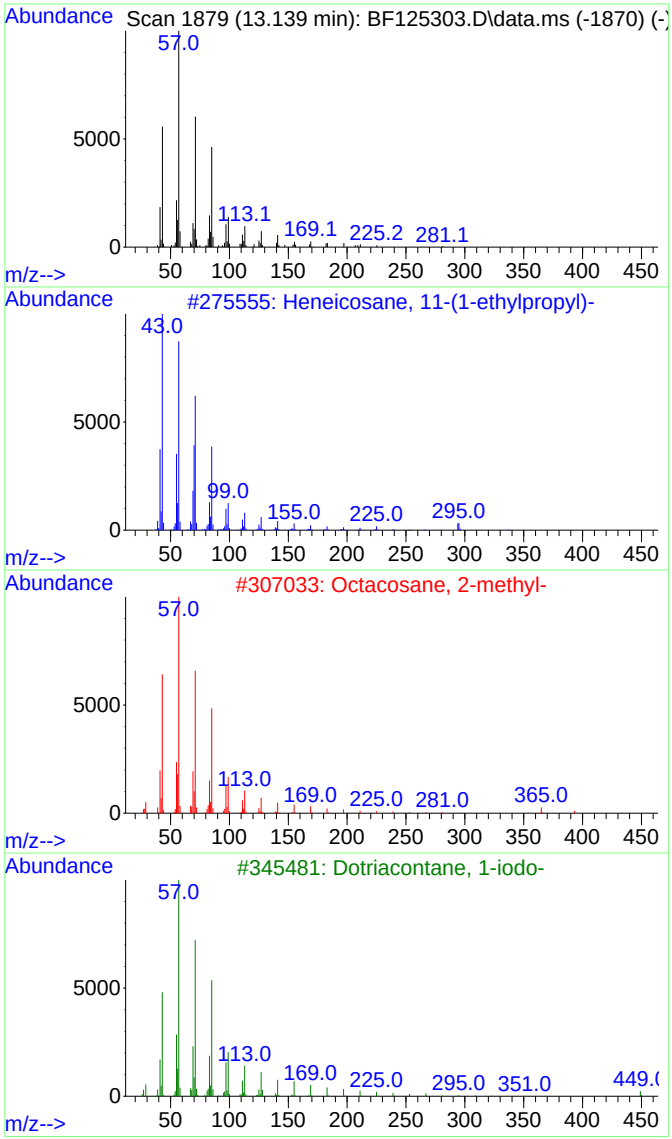
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

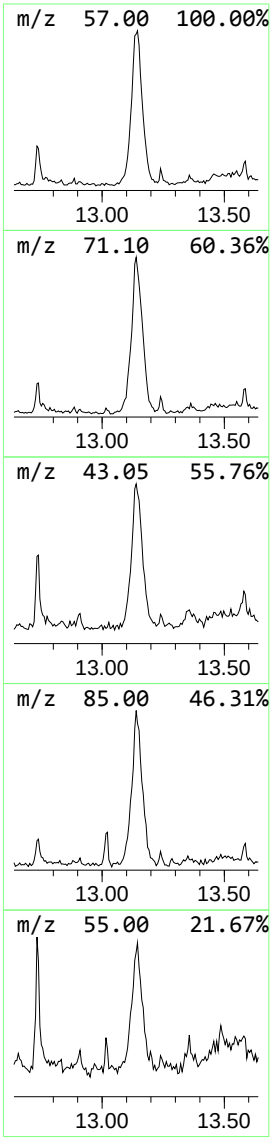
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Heneicosane, 11-(1-ethylpro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.139	6.61 ng	547742	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5	Pentadecane, 7-(bromomethyl)-	304	C16H33Br	052997-43-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125303.D
Acq On : 1 Sep 2021 13:24
Operator : JU/CG
Sample : M3612-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-1

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

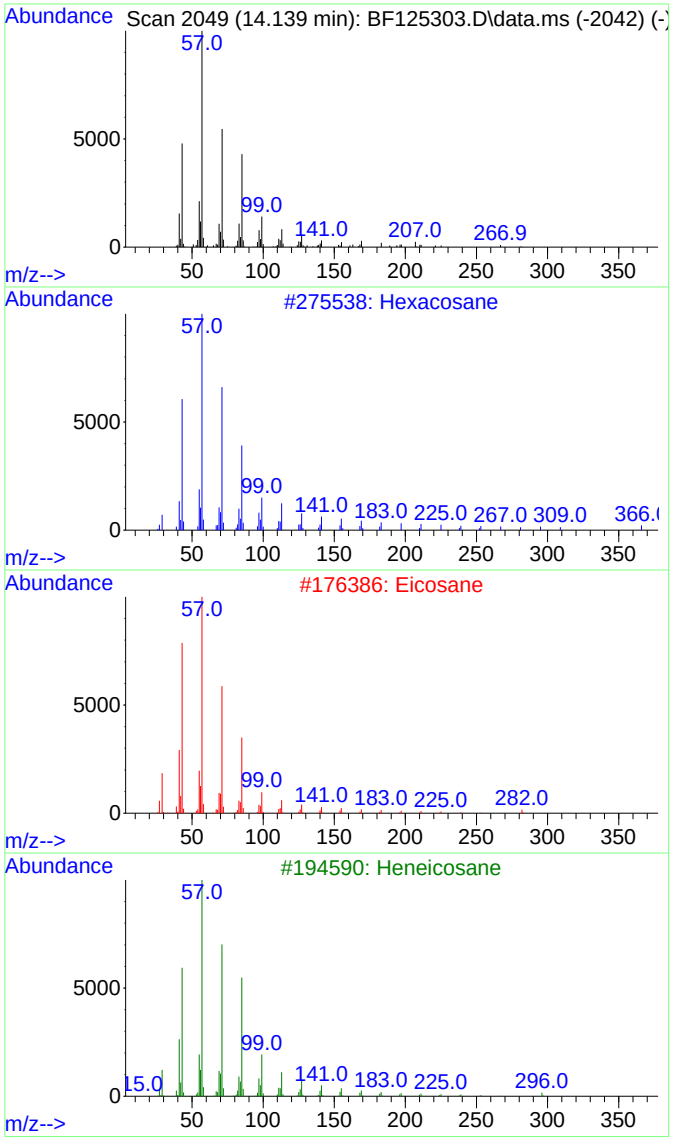
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

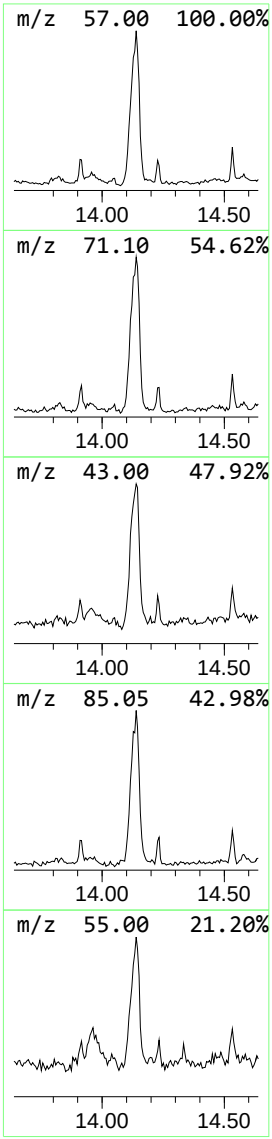
****

Peak Number 5 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.139	5.66 ng	468374	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Eicosane	282	C20H42	000112-95-8	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Octadecane	254	C18H38	000593-45-3	87
5	Hexadecane	226	C16H34	000544-76-3	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125303.D
Acq On : 1 Sep 2021 13:24
Operator : JU/CG
Sample : M3612-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-1

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

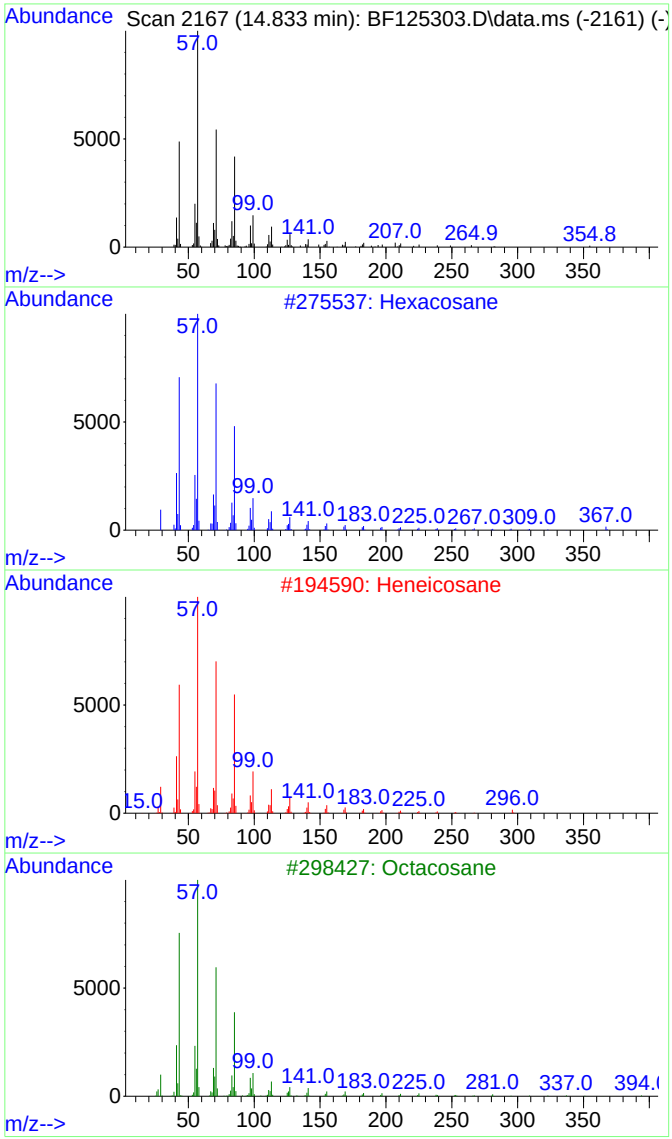
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

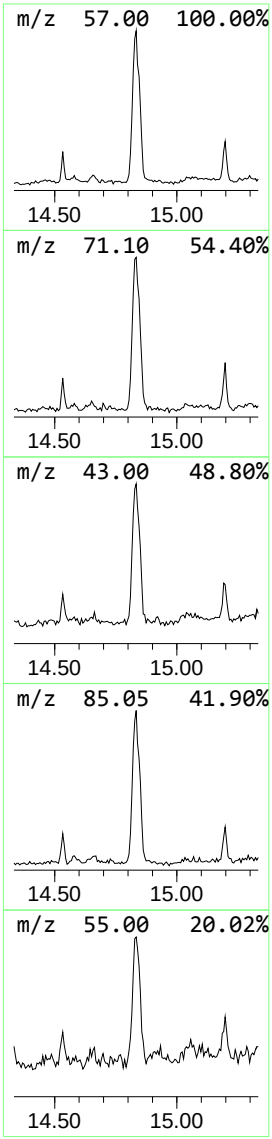
****

Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	5.22 ng	466847	Perylene-d12	15.574

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	Octacosane	394	C28H58	000630-02-4	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Tetratetracontane	619	C44H90	007098-22-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125303.D
Acq On : 1 Sep 2021 13:24
Operator : JU/CG
Sample : M3612-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
M-1

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

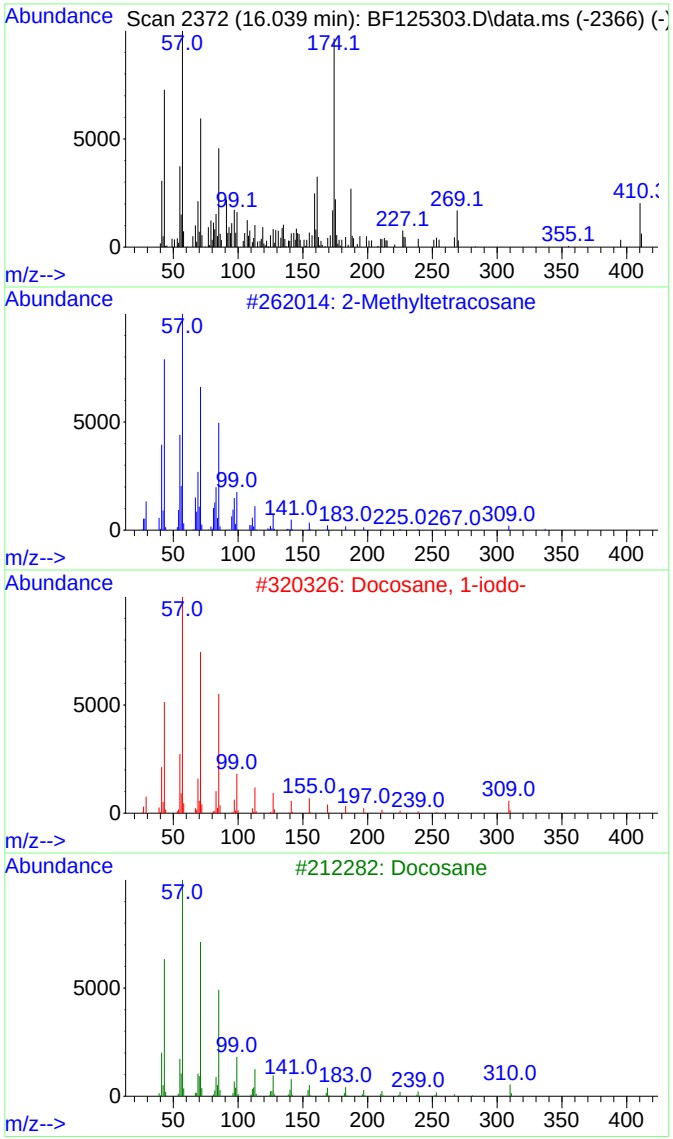
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

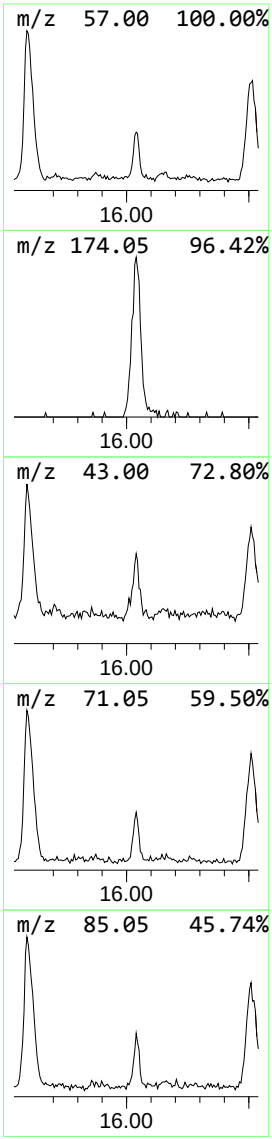
****

Peak Number 7 unknown16.039 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.039	3.32 ng	296551	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyltetracosane	352	C25H52	001560-78-7	20
2	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	20
3	Docosane	310	C22H46	000629-97-0	20
4	Pentacosane	352	C25H52	000629-99-2	20
5	Heneicosane	296	C21H44	000629-94-7	20





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125303.D
Acq On : 1 Sep 2021 13:24
Operator : JU/CG
Sample : M3612-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-1

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

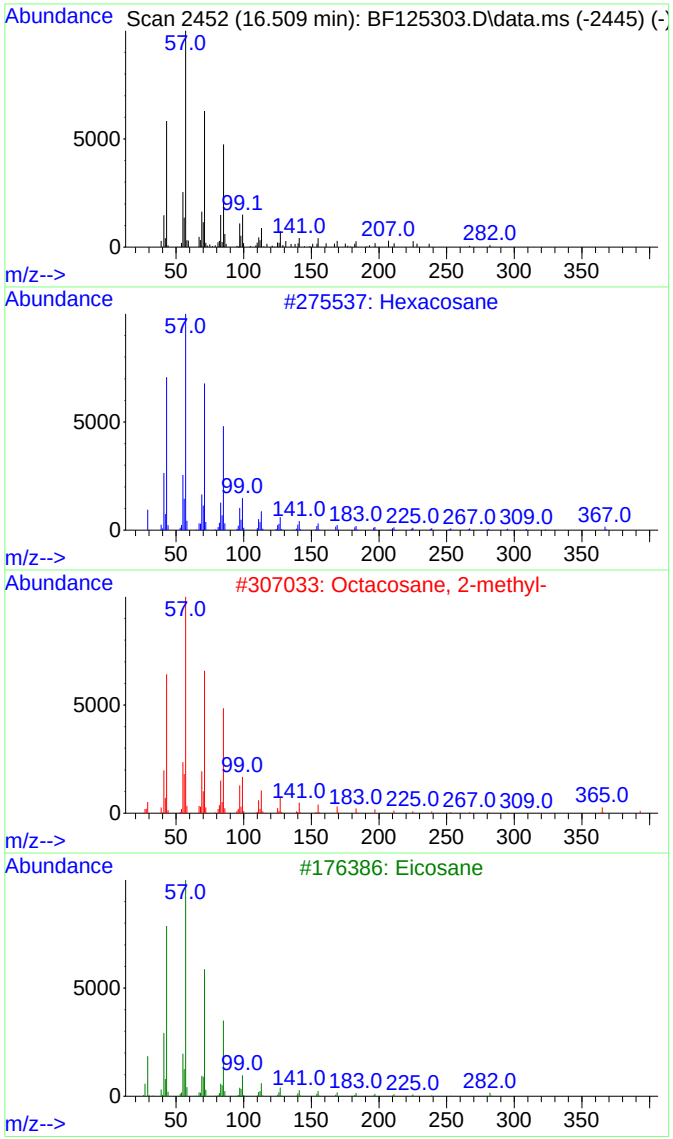
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

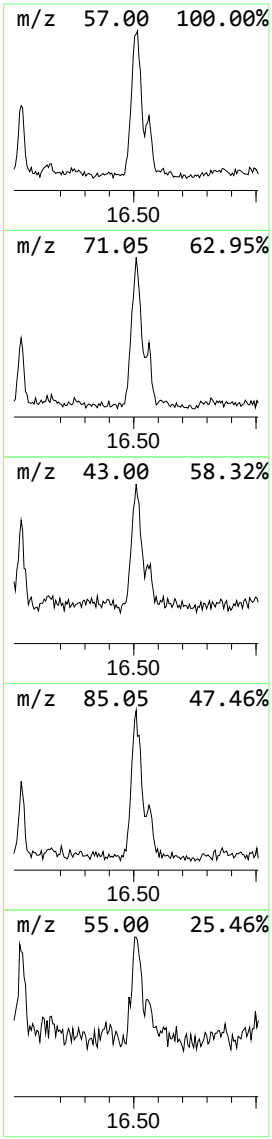
****

Peak Number 8 Octacosane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.509	3.16 ng	282544	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Eicosane	282	C20H42	000112-95-8	91
4	Hexatriacontane	507	C36H74	000630-06-8	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125303.D
Acq On : 1 Sep 2021 13:24
Operator : JU/CG
Sample : M3612-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-1

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

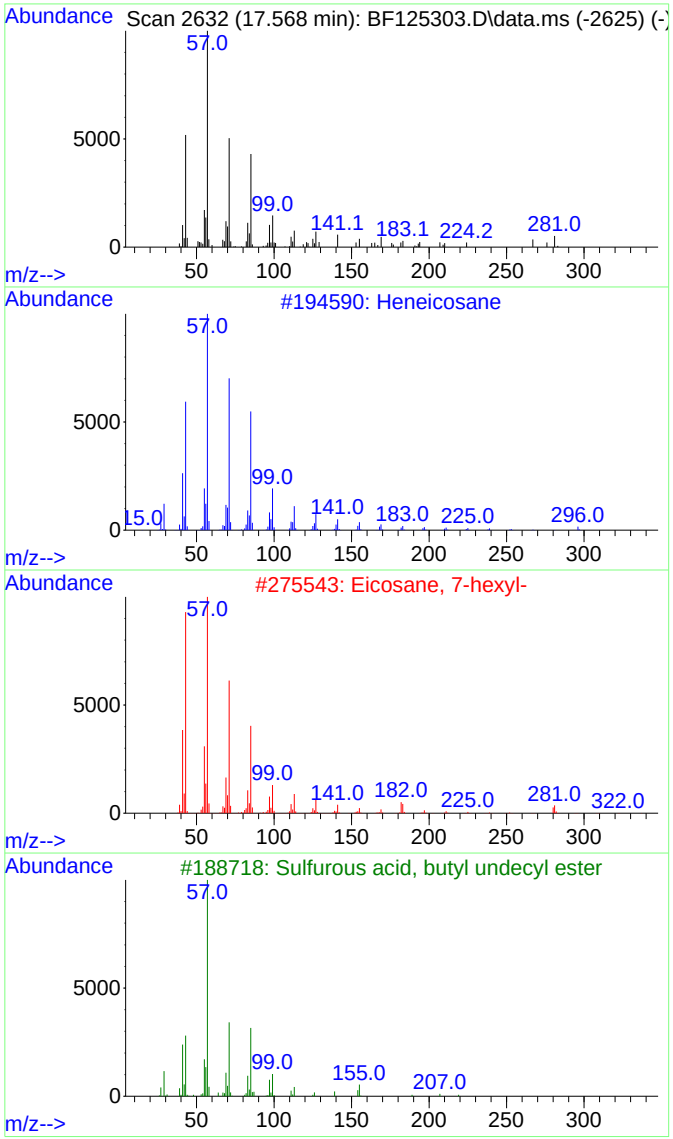
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

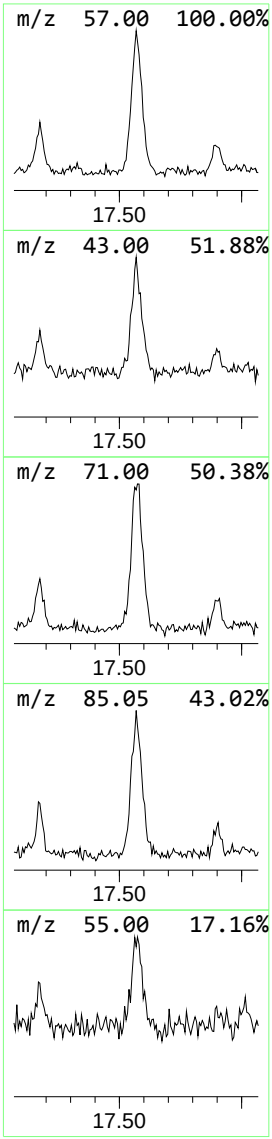
****

Peak Number 9 Eicosane, 7-hexyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.568	2.77 ng	247330	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86
3	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	83
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	83
5	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125303.D
Acq On : 1 Sep 2021 13:24
Operator : JU/CG
Sample : M3612-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-1

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

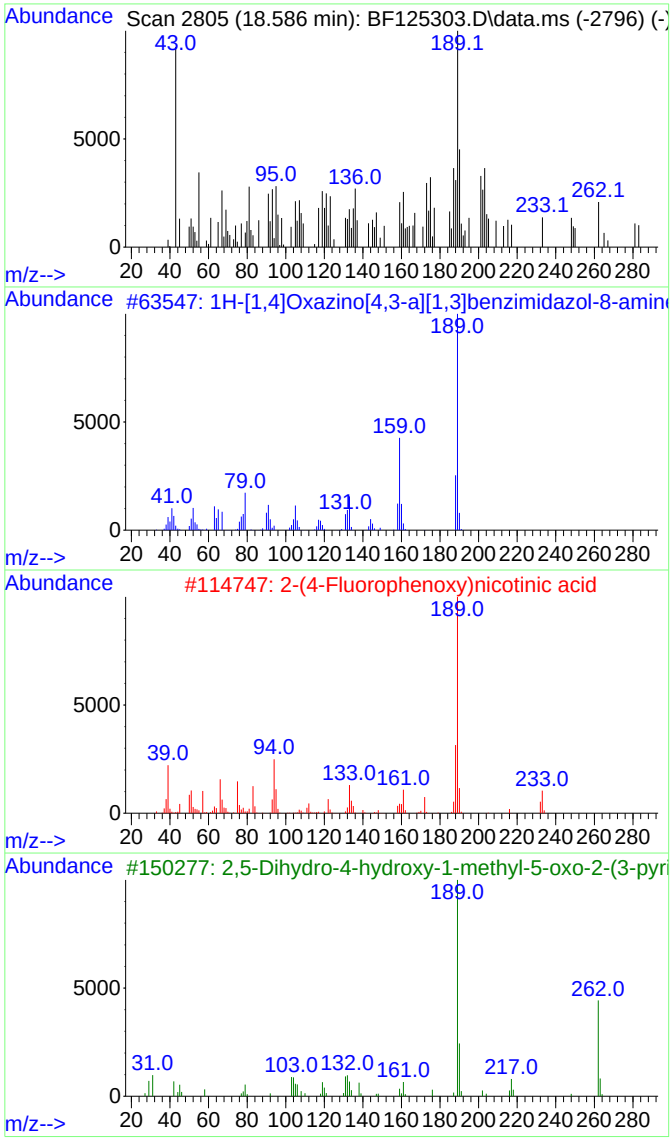
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

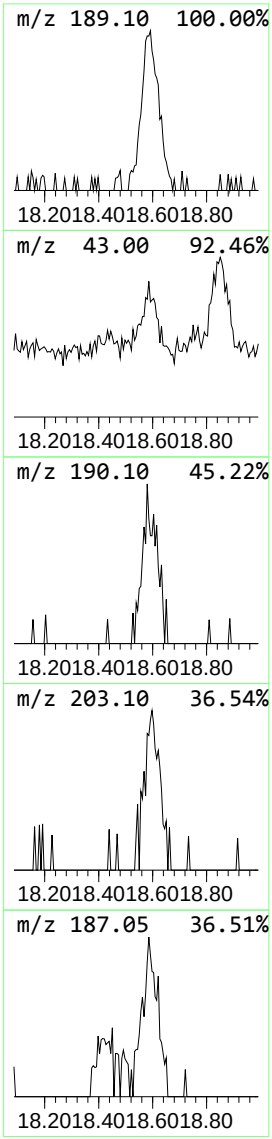
****

Peak Number 10 unknown18.586 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.586	3.03 ng	271182	Perylene-d12	15.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-[1,4]Oxazino[4,3-a][1,3]benzi...	189	C10H11N3O	1000362-54-6	42
2	2-(4-Fluorophenoxy)nicotinic acid	233	C12H8FNO3	054629-13-9	38
3	2,5-Dihydro-4-hydroxy-1-methyl-5...	262	C13H14N2O4	1000434-41-3	38
4	9-Methyltetracyclo[7.3.1.0(2.7)....	204	C15H24	1000215-30-5	30
5	N-[1-(2-Methylphenyl)ethyl]-4,5-...	204	C12H16N2O	101932-32-5	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090121\
Data File : BF125303.D
Acq On : 1 Sep 2021 13:24
Operator : JU/CG
Sample : M3612-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : M-1

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...	2.163	22.8	ng	1225010	1	6.904	1073020	20.0
Ethanol, 2-(2-b...	8.092	6.4	ng	459682	2	8.187	1443270	20.0
n-Hexadecanoic ...	11.951	5.5	ng	523438	4	11.433	1885530	20.0
Heneicosane, 11...	13.139	6.6	ng	547742	5	14.074	1656440	20.0
Hexacosane	14.139	5.7	ng	468374	5	14.074	1656440	20.0
Heneicosane	14.833	5.2	ng	466847	6	15.574	1788420	20.0
unknown16.039	16.039	3.3	ng	296551	6	15.574	1788420	20.0
Octacosane, 2-m...	16.509	3.2	ng	282544	6	15.574	1788420	20.0
Eicosane, 7-hexyl-	17.568	2.8	ng	247330	6	15.574	1788420	20.0
unknown18.586	18.586	3.0	ng	271182	6	15.574	1788420	20.0