LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128573.D
Acq On : 29 May 2022 16:03
Operator : CG\JU
Sample : N2951-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-01

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-BF052622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128573.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.057	467	471	477	rVB	37316	45759	1.67%	0.209%
2	5.451	532	538	541	rBV	2921612	2738833	99.74%	12.482%
3	5.675	571	576	582	rVB2	31100	29217	1.06%	0.133%
4	6.463	704	710	713	rBV	2625652	2585652	94.16%	11.784%
5	6.575	726	729	734	rBV	44808	44504	1.62%	0.203%
6	6.839	770	774	779	rVB	802820	707456	25.76%	3.224%
7	7.110	815	820	824	rBV2	25033	30975	1.13%	0.141%
8	7.239	837	842	844	rBV3	22269	28495	1.04%	0.130%
9	7.398	864	869	872	rBV	2020479	1783805	64.96%	8.130%
10	7.434	872	875	879	rVB	28984	28843	1.05%	0.131%
11	7.469	879	881	886	rVB4	34566	47609	1.73%	0.217%
12	8.116	986	991	995	rBV	886198	783127	28.52%	3.569%
13	9.198	1170	1175	1178	rBV	2969763	2746054	100.00%	12.515%
14	9.875	1286	1290	1293	rBV	977730	789360	28.75%	3.598%
15	10.663	1419	1424	1427	rBV	1951908	1716806	62.52%	7.824%
16	11.139	1501	1505	1508	rVB	45244	37513	1.37%	0.171%
17	11.357	1539	1542	1546	rBV	820872	759274	27.65%	3.460%
18	11.892	1629	1633	1644	rBV	393866	415158	15.12%	1.892%
19	12.598	1751	1753	1759	rVB4	26103	29263	1.07%	0.133%
20	12.674	1763	1766	1776	rBV2	145689	163772	5.96%	0.746%
21	12.951	1808	1813	1816	rBV	2940969	2566249	93.45%	11.696%
22	13.427	1891	1894	1898	rVB	41157	37566	1.37%	0.171%
23	13.810	1954	1959	1963	rBV	136972	138908	5.06%	0.633%
24	13.874	1965	1970	1983	rBV	159347	362639	13.21%	1.653%
25	13.998	1986	1991	1995	rBV2	964630	1114259	40.58%	5.078%
26	14.098	2004	2008	2012	rBV	331076	338890	12.34%	1.544%
27	14.139	2012	2015	2018	rVV	165590	137869	5.02%	0.628%
28	14.180	2018	2022	2024	rVV2	256094	227435	8.28%	1.037%
29	14.210	2024	2027	2029	rVV	78649	80607	2.94%	0.367%
30	14.227	2029	2030	2033	rVB	83219	65941	2.40%	0.301%
31	14.480	2070	2073	2076	rBV	45412	37919	1.38%	0.173%
32	14.521	2077	2080	2086	rVV3	59562	70953	2.58%	0.323%
33	14.768	2119	2122	2123	rBV	39141	37490	1.37%	0.171%
34	14.786	2123	2125	2130	rVB	48612	48934	1.78%	0.223%
35	15.127	2180	2183	2189	rVB	60920	68361	2.49%	0.312%
36	15.462	2236	2240	2245	rBV	645338	815161	29.68%	3.715%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
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Operator : CG\JU
Sample : N2951-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-01

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-BF052622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.509	2245	2248	2253	rVB	62875	79720	2.90%	0.363%
38	15.945	2319	2322	2328	rBV2	44166	63111	2.30%	0.288%
39	16.456	2404	2409	2420	rVB2	42574	94257	3.43%	0.430%
40	17.045	2507	2509	2517	rVB5	26404	44132	1.61%	0.201%

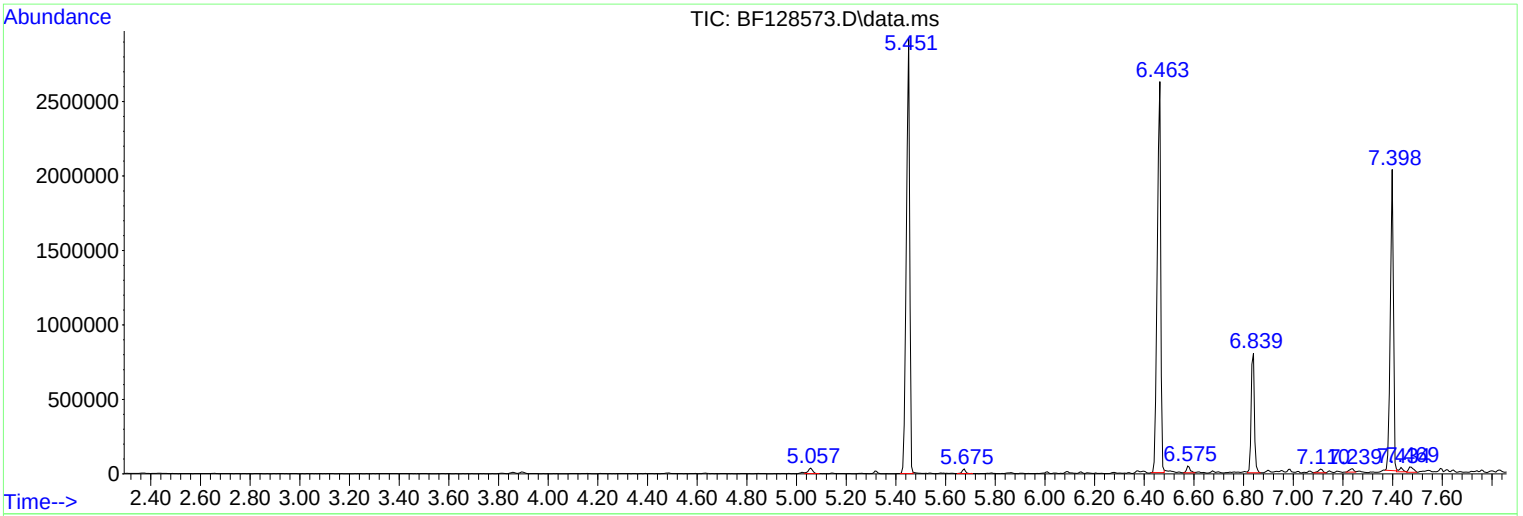
Sum of corrected areas: 21941876

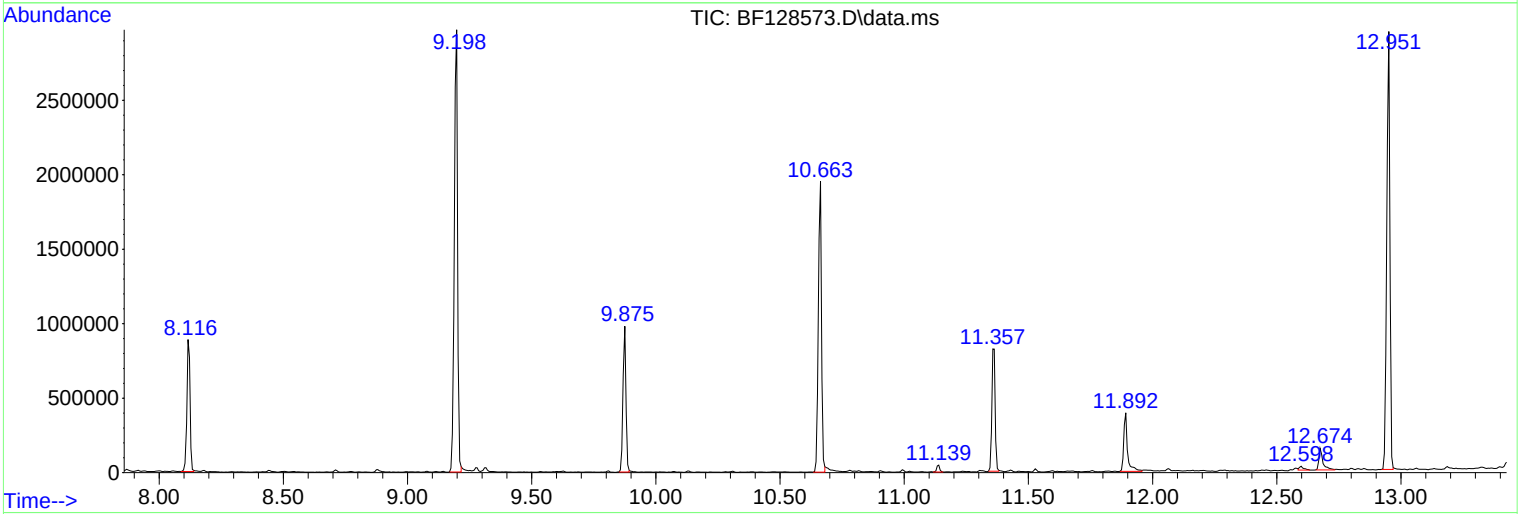
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128573.D
Acq On : 29 May 2022 16:03
Operator : CG\JU
Sample : N2951-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

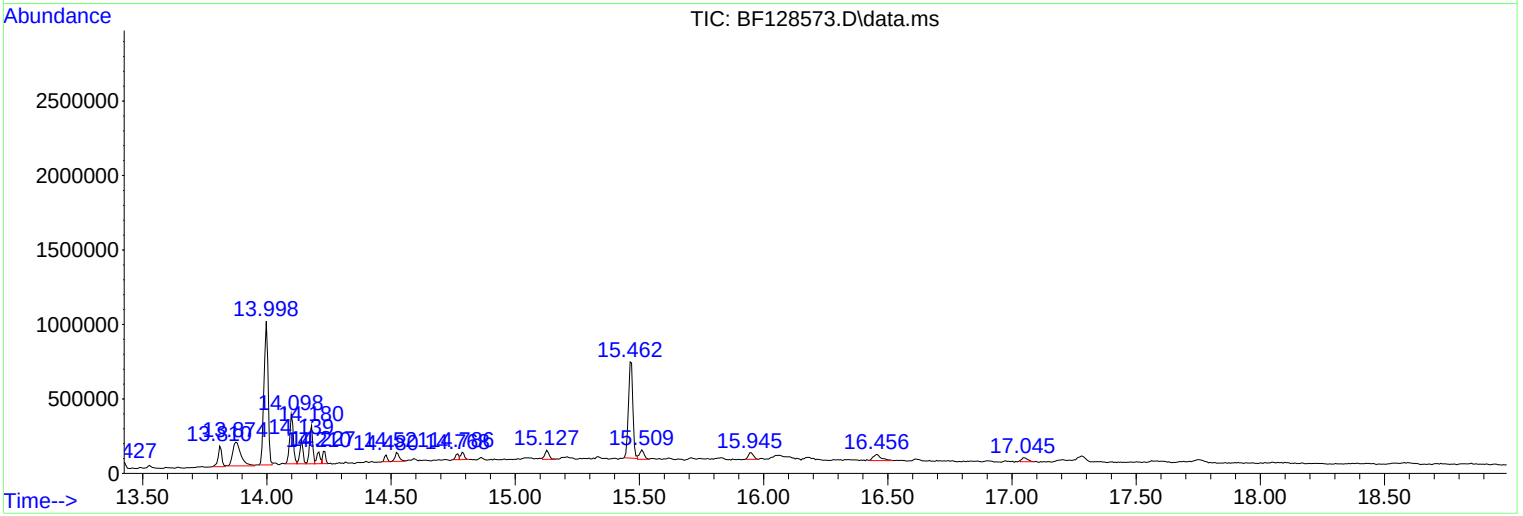
Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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\BF052922\
Data File : BF128573.D
Acq On : 29 May 2022 16:03
Operator : CG\JU
Sample : N2951-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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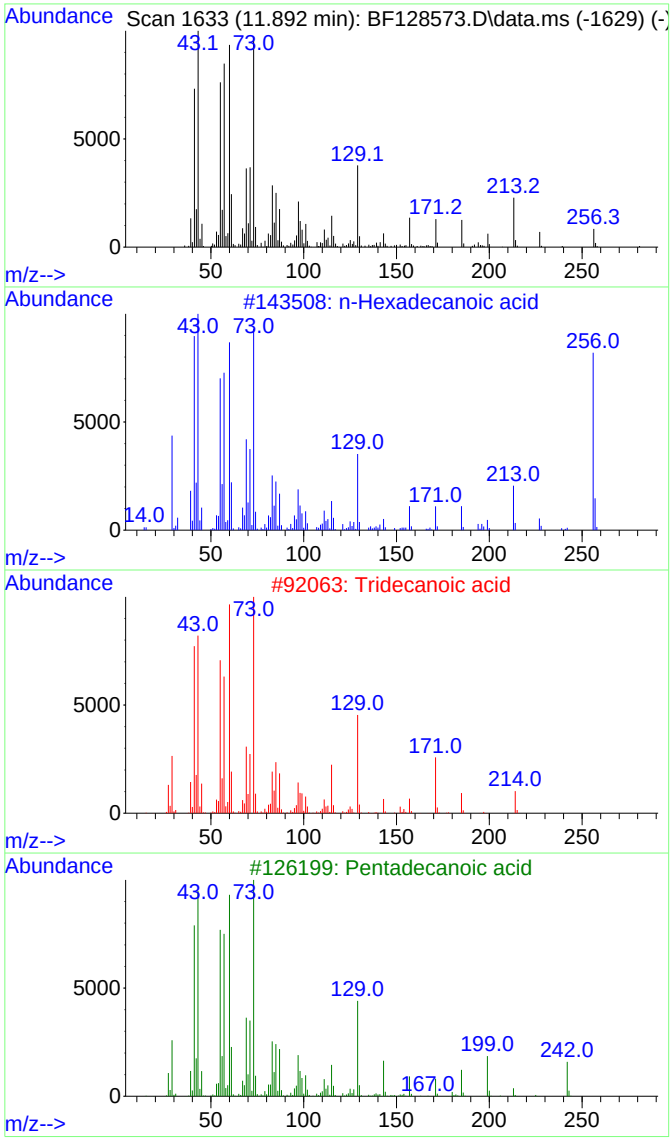
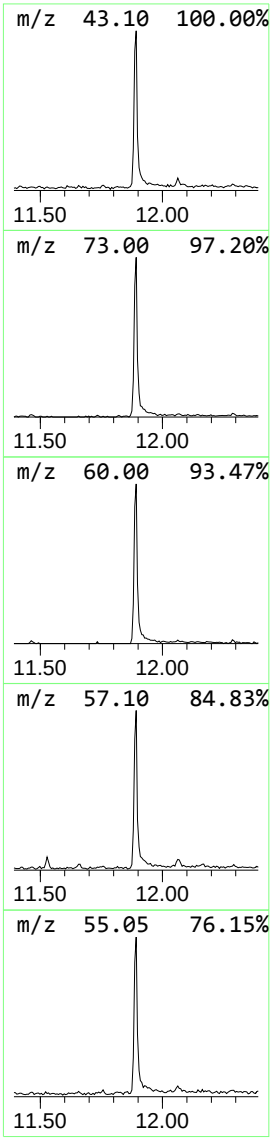
Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	10.94 ng	415158	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128573.D
Acq On : 29 May 2022 16:03
Operator : CG\JU
Sample : N2951-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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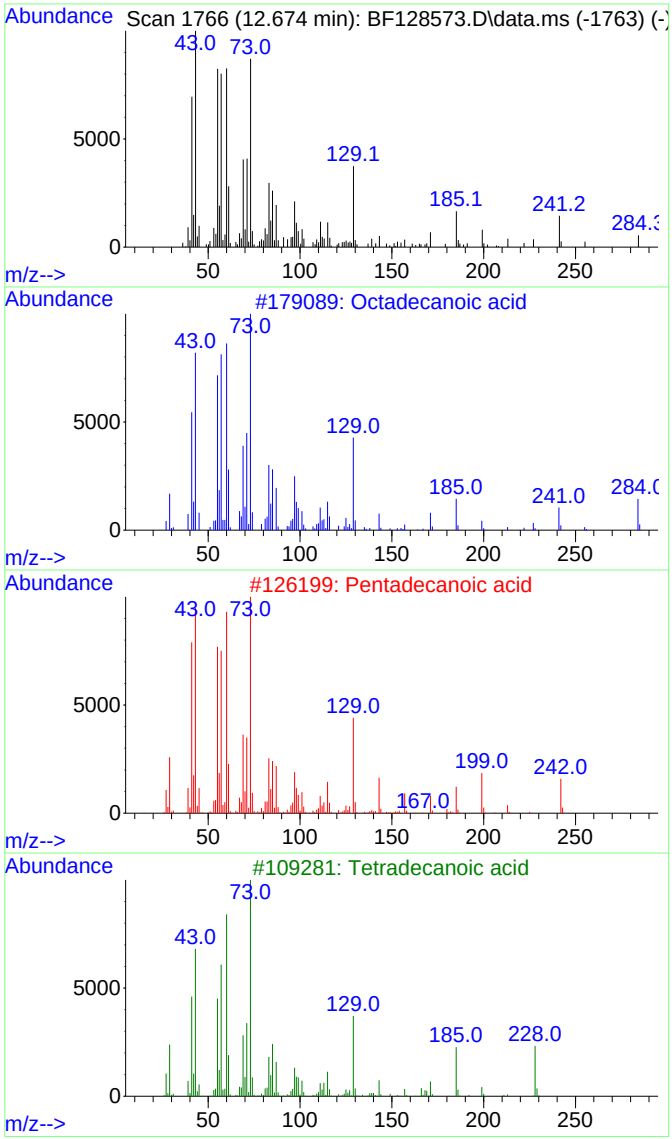
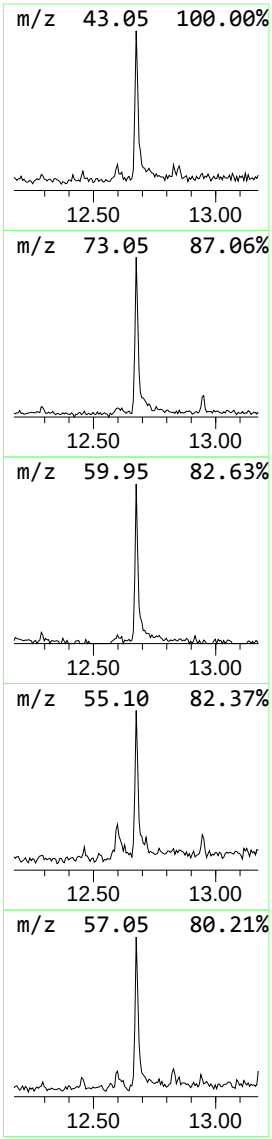
Peak Number 2 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.674	4.31 ng	163772	Phenanthrene-d10	11.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Undecanoic acid	186	C11H22O2	000112-37-8	46
5	Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128573.D
Acq On : 29 May 2022 16:03
Operator : CG\JU
Sample : N2951-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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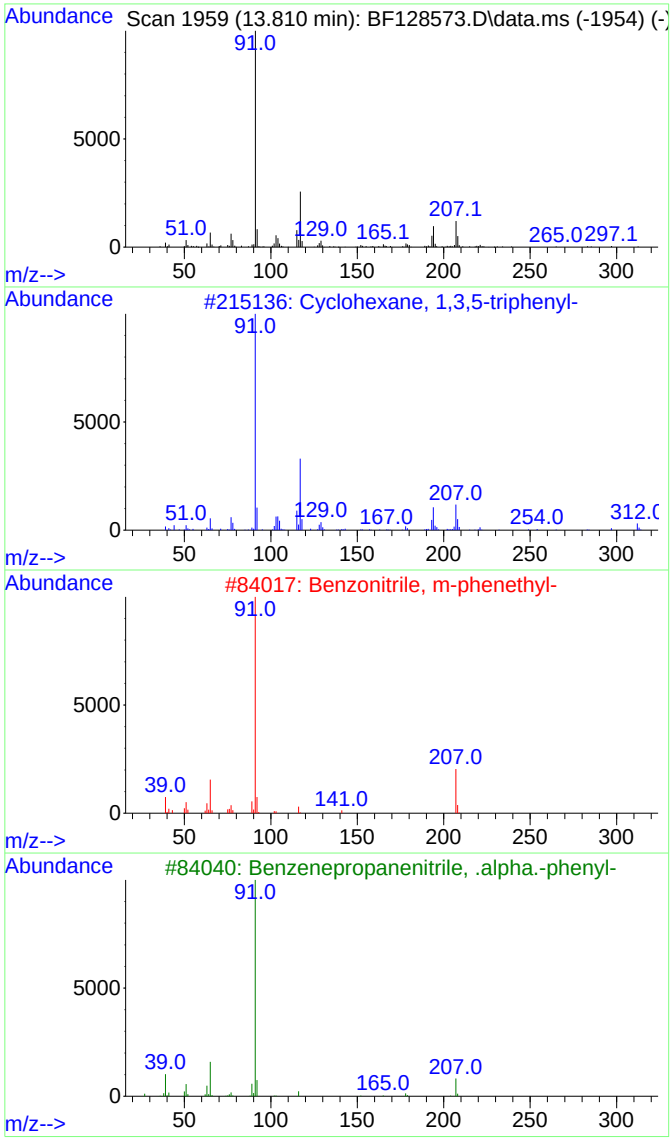
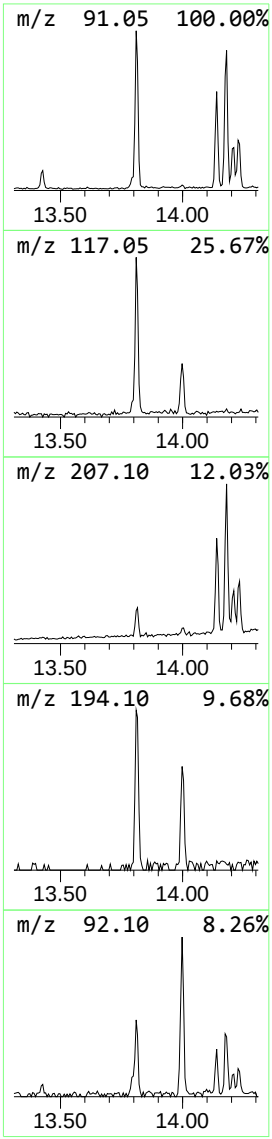
Peak Number 3 Cyclohexane, 1,3,5-triphenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	2.49 ng	138908	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3,5-triphenyl-	312	C24H24	028336-57-4	83
2	Benzonitrile, m-phenethyl-	207	C15H13N	034176-91-5	27
3	Benzenepropanenitrile, .alpha.-p...	207	C15H13N	003333-14-0	27
4	2-Propenoic acid, 3-[(phenylmeth...	194	C10H10O2S	013831-01-1	25
5	Bendazac methyl ester	296	C17H16N2O3	1010119-77-6	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128573.D
Acq On : 29 May 2022 16:03
Operator : CG\JU
Sample : N2951-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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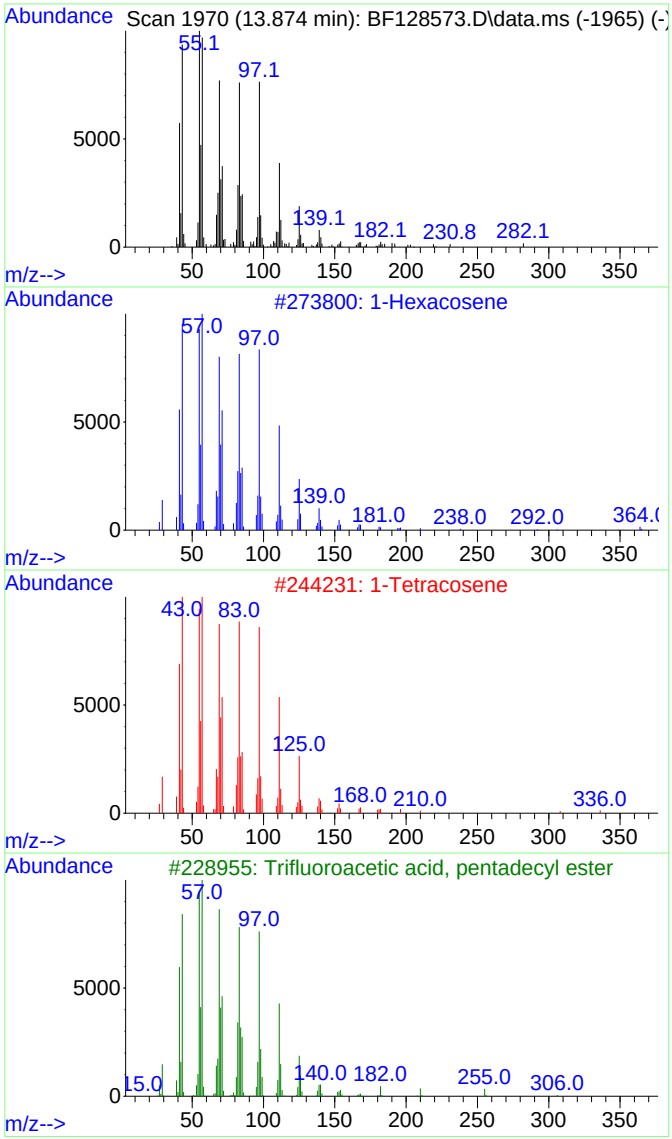
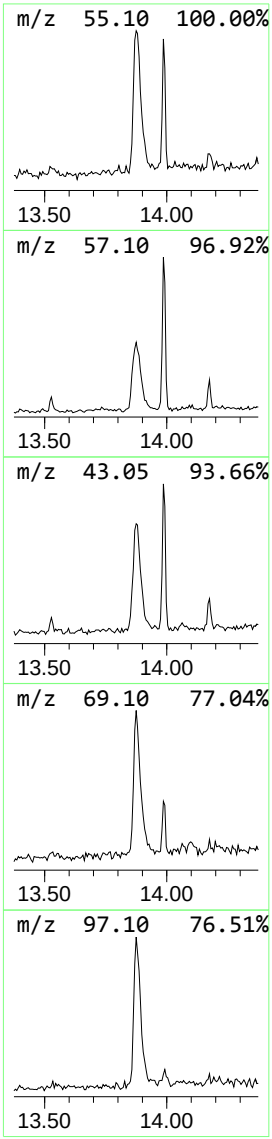
Peak Number 4 1-Hexacosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	6.51 ng	362639	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	94
2	1-Tetracosene	336	C24H48	010192-32-2	91
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128573.D
Acq On : 29 May 2022 16:03
Operator : CG\JU
Sample : N2951-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

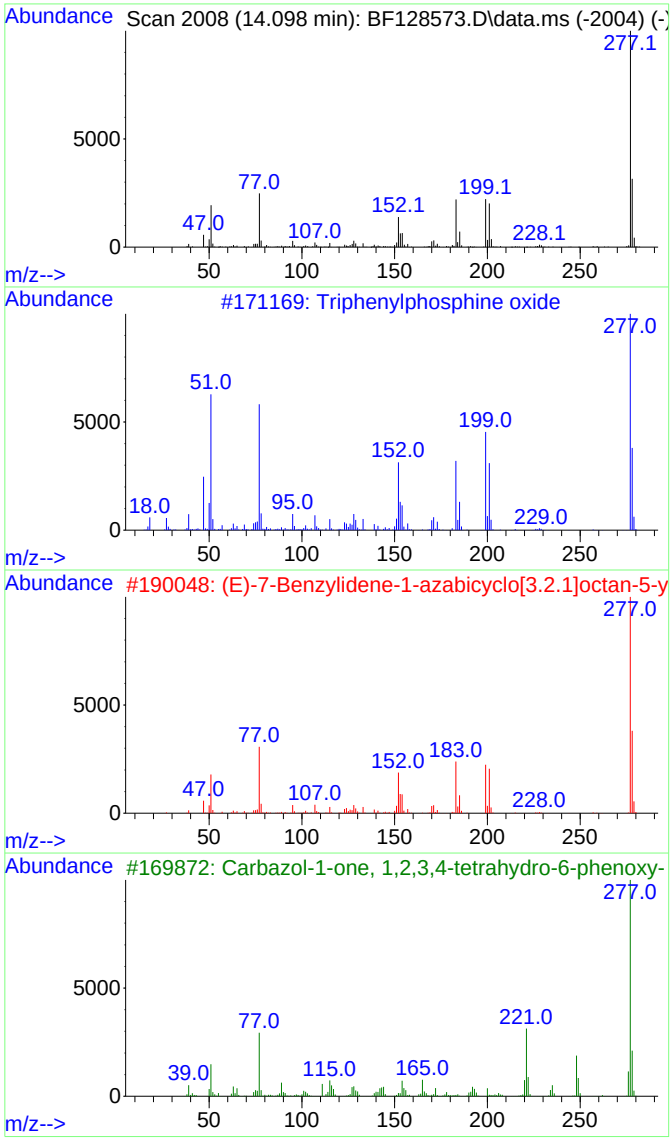
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

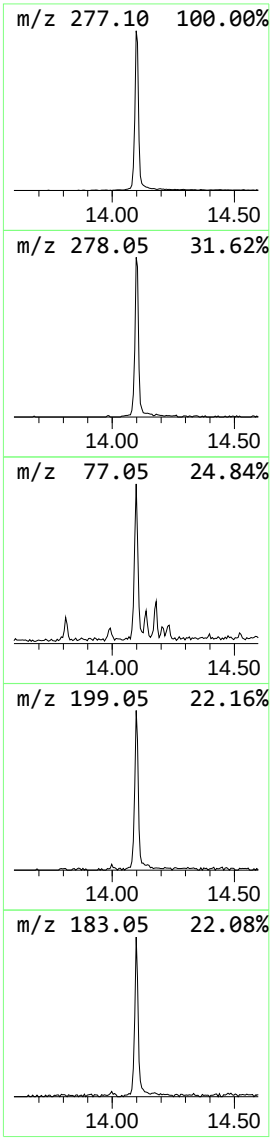
****

Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	6.08 ng	338890	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	49
3	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	37
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	33
5	2-Propenoic acid, 2-cyano-3-(3-p...	277	C18H15NO2	1000080-00-3	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128573.D
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Sample : N2951-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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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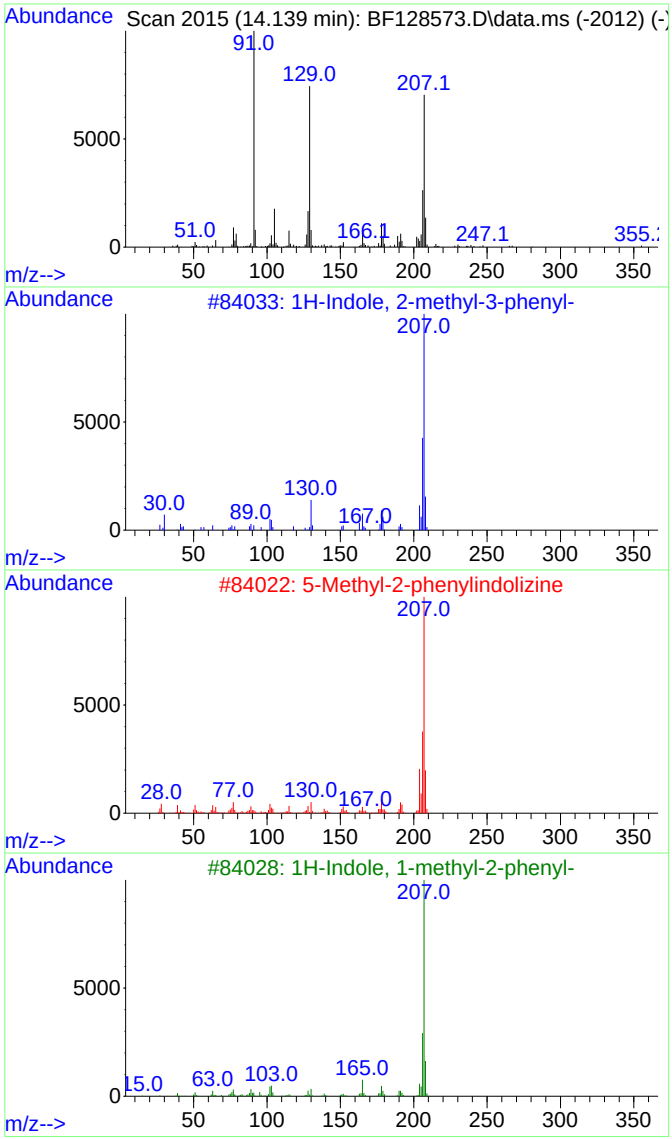
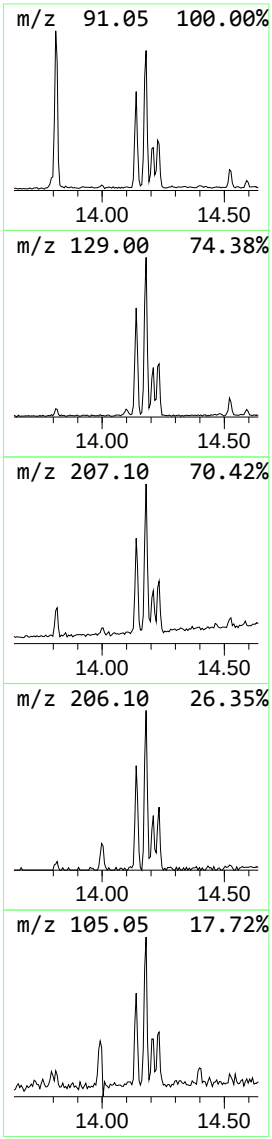
Peak Number 6 unknown14.139 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.139	2.47 ng	137869	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	42
2	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	42
3	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	38
4	Methadone N-oxide	325	C21H27NO2	1000120-80-7	38
5	Quinoline-8-carboxylic acid	173	C10H7NO2	000086-59-9	35





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

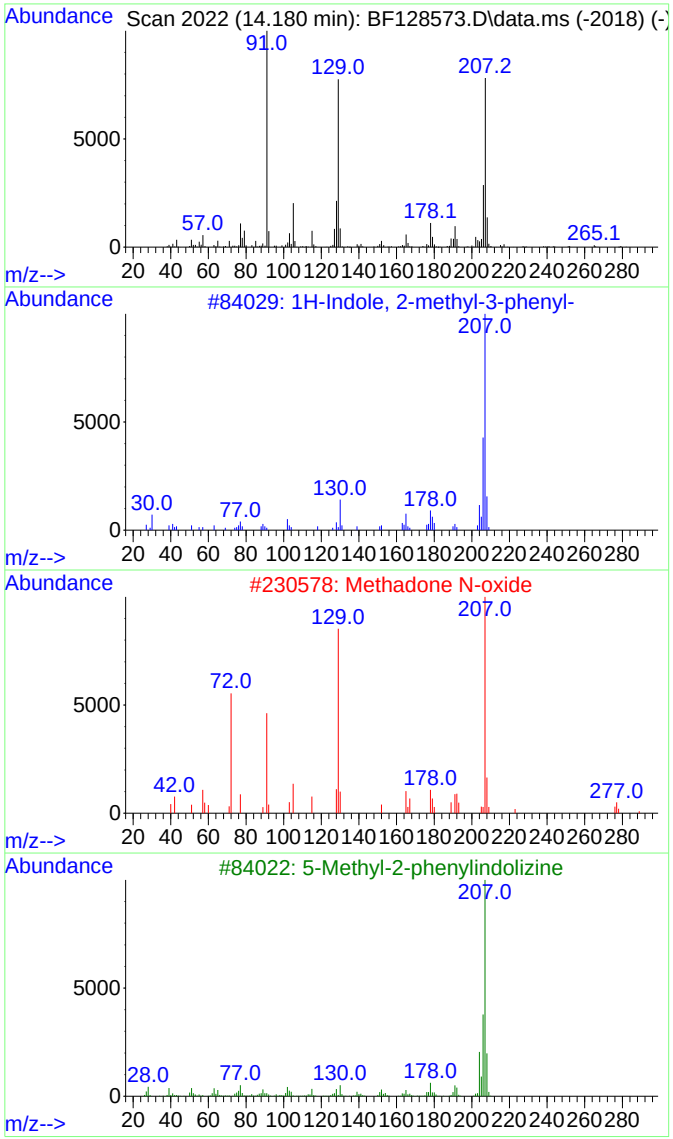
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

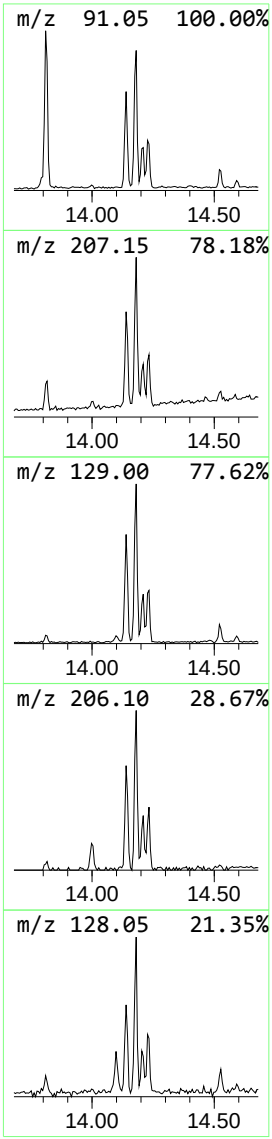
****

Peak Number 7 unknown14.180 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.180	4.08 ng	227435	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	46
2	Methadone N-oxide	325	C21H27NO2	1000120-80-7	45
3	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	43
4	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1010154-23-3	38
5	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128573.D
Acq On : 29 May 2022 16:03
Operator : CG\JU
Sample : N2951-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-01

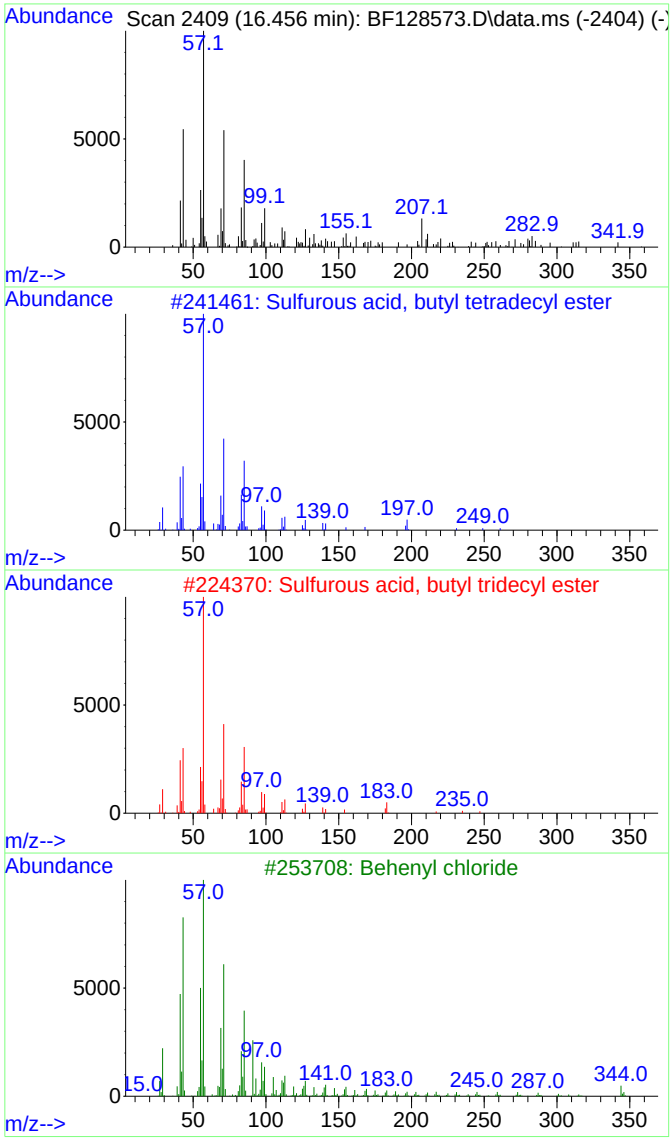
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

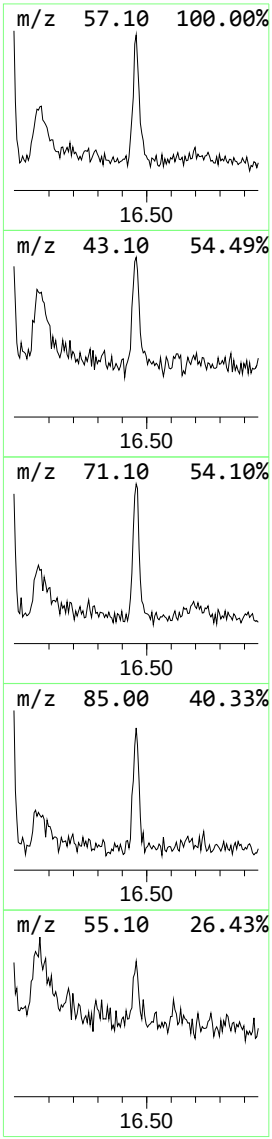
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Sulfurous acid, butyl tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.456	2.31 ng	94257	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	72
2	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	72
3	Behenyl chloride	344	C22H45Cl	042217-03-8	64
4	Docosane, 7-butyl-	366	C26H54	055282-15-0	64
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052922\
Data File : BF128573.D
Acq On : 29 May 2022 16:03
Operator : CG\JU
Sample : N2951-18
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P036-SS001-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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
n-Hexadecanoic ...	11.892	10.9	ng	415158	4	11.363	759274	20.0
Octadecanoic acid	12.674	4.3	ng	163772	4	11.363	759274	20.0
Cyclohexane, 1,...	13.810	2.5	ng	138908	5	13.998	1114260	20.0
1-Hexacosene	13.874	6.5	ng	362639	5	13.998	1114260	20.0
Triphenylphosph...	14.098	6.1	ng	338890	5	13.998	1114260	20.0
unknown14.139	14.139	2.5	ng	137869	5	13.998	1114260	20.0
unknown14.180	14.180	4.1	ng	227435	5	13.998	1114260	20.0
Sulfurous acid,...	16.456	2.3	ng	94257	6	15.468	815161	20.0