LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123959.D
Acq On : 17 May 2021 12:56
Operator : JU/CG
Sample : M2322-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3-20210505

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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123959.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	8	16	21	rVB	2159076	2840398	100.00%	17.949%
2	2.287	30	34	38	rBV	36264	45892	1.62%	0.290%
3	5.510	578	582	586	rBV	687053	640732	22.56%	4.049%
4	6.516	749	753	758	rBV	480991	409053	14.40%	2.585%
5	6.904	815	819	822	rVB	365490	283276	9.97%	1.790%
6	7.463	909	914	917	rBV	1088114	980622	34.52%	6.197%
7	8.187	1033	1037	1040	rBV	467624	364171	12.82%	2.301%
8	9.263	1215	1220	1223	rBV	2140672	1748323	61.55%	11.048%
9	9.939	1332	1335	1339	rBV	528957	435328	15.33%	2.751%
10	10.369	1402	1408	1411	rBV	2884213	2714646	95.57%	17.155%
11	10.733	1465	1470	1473	rBV	1483483	1247213	43.91%	7.881%
12	11.427	1584	1588	1592	rBV	610913	479225	16.87%	3.028%
13	11.957	1674	1678	1688	rVB2	179817	225016	7.92%	1.422%
14	12.410	1751	1755	1757	rBV2	42069	36863	1.30%	0.233%
15	12.739	1808	1811	1818	rBV2	122644	124775	4.39%	0.788%
16	13.021	1854	1859	1862	rBV	2024064	1993290	70.18%	12.596%
17	13.916	2007	2011	2020	rBV	236699	248572	8.75%	1.571%
18	14.068	2033	2037	2040	rBV	496984	411188	14.48%	2.598%
19	14.551	2113	2119	2123	rVB8	20781	31991	1.13%	0.202%
20	15.210	2227	2231	2236	rBV	27122	33977	1.20%	0.215%
21	15.563	2285	2291	2295	rBV2	284109	341303	12.02%	2.157%
22	15.604	2295	2298	2303	rVB2	29621	37897	1.33%	0.239%
23	16.057	2368	2375	2380	rBV2	24314	39209	1.38%	0.248%
24	16.110	2380	2384	2393	rVV4	22012	36594	1.29%	0.231%
25	16.580	2457	2464	2469	rBV2	21787	39581	1.39%	0.250%
26	17.198	2561	2569	2573	rBV7	14439	35504	1.25%	0.224%

Sum of corrected areas: 15824639

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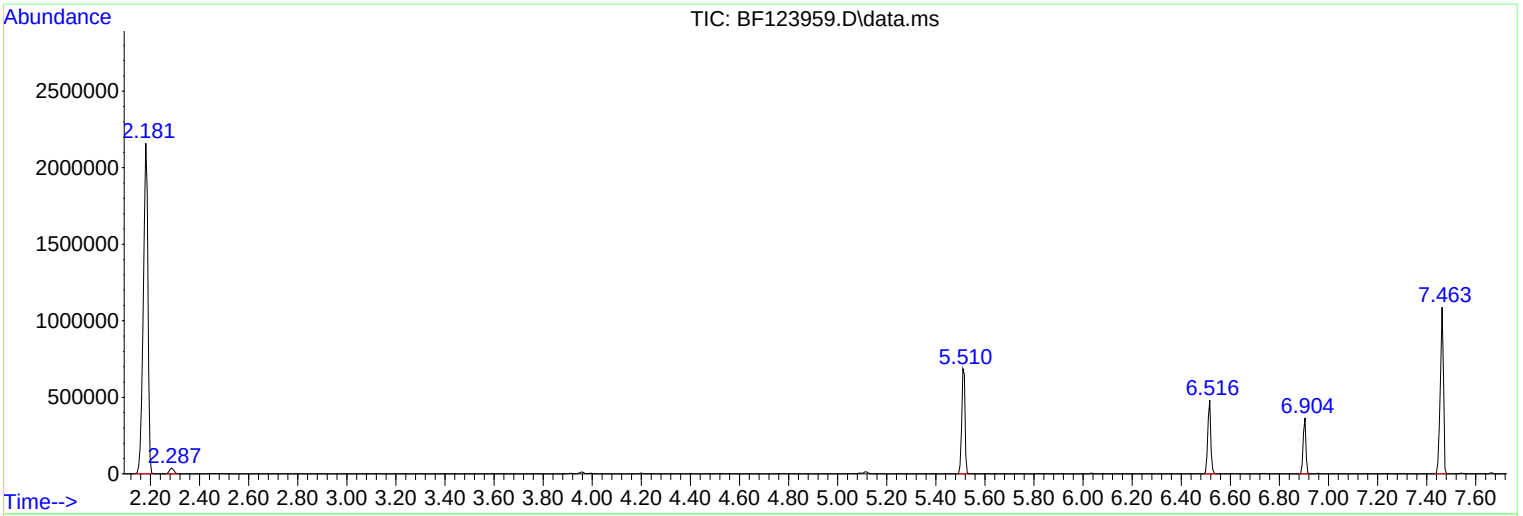
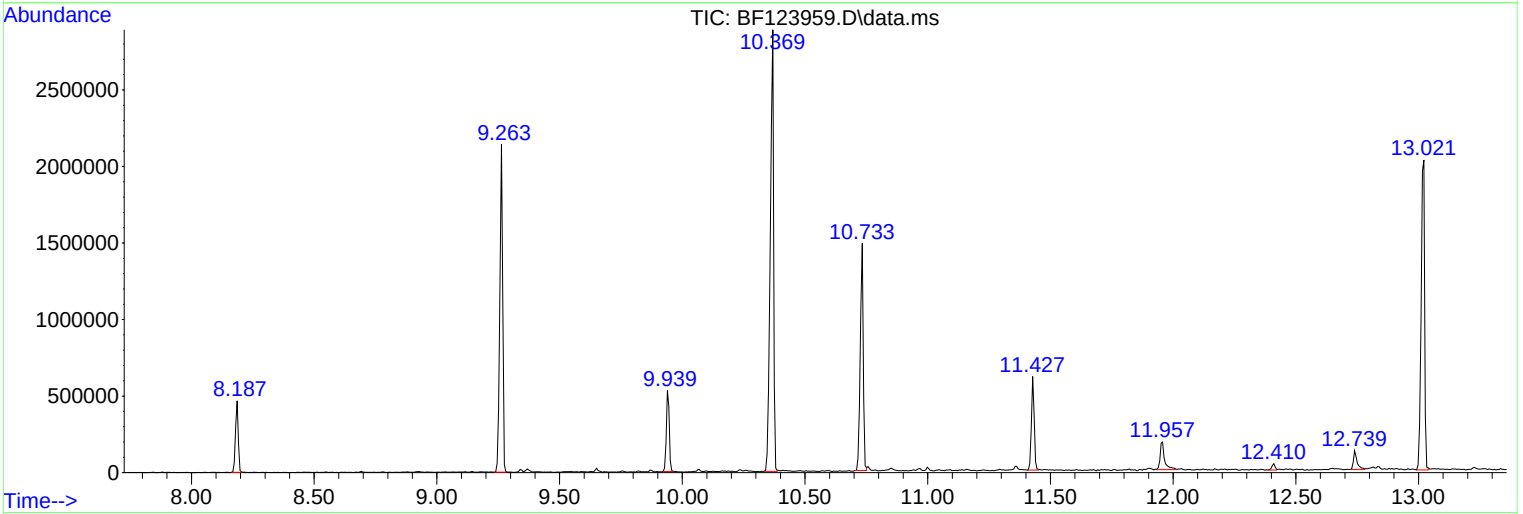
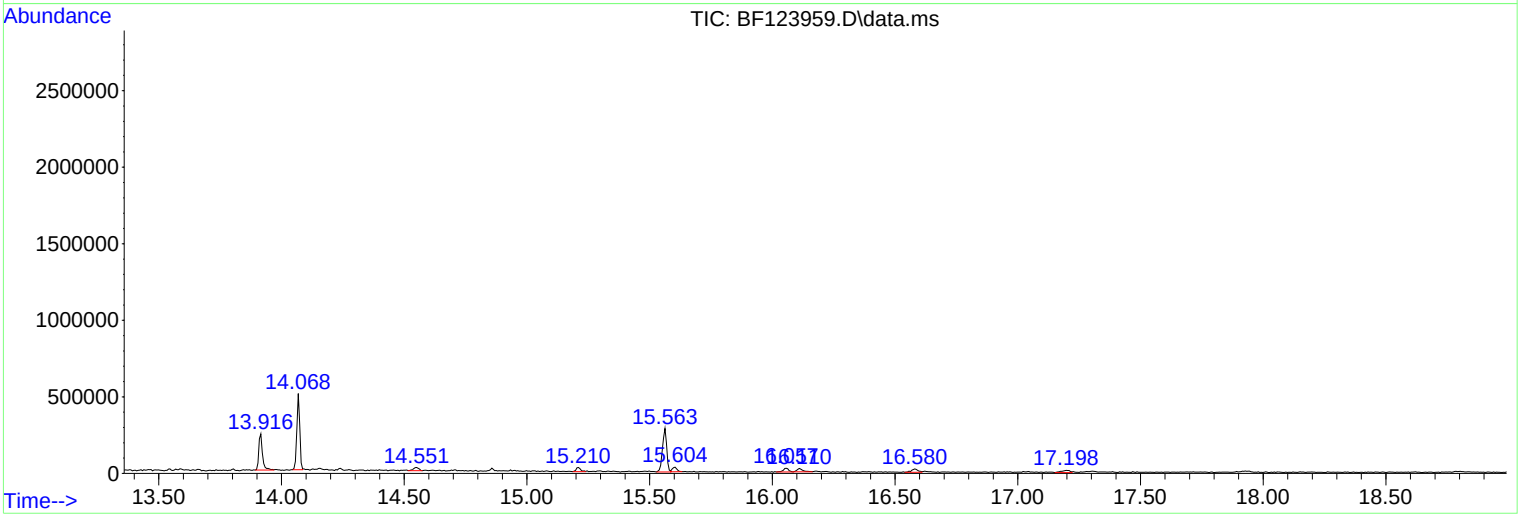
Instrument :
BNA_F
ClientSampleId :
MW-3-20210505

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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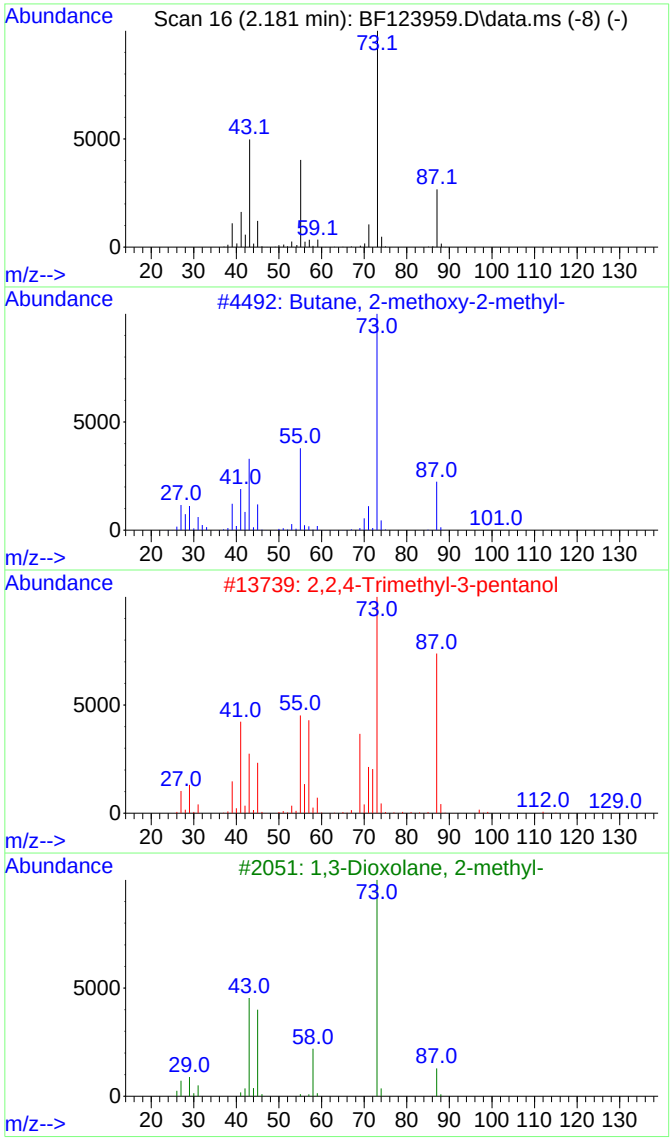
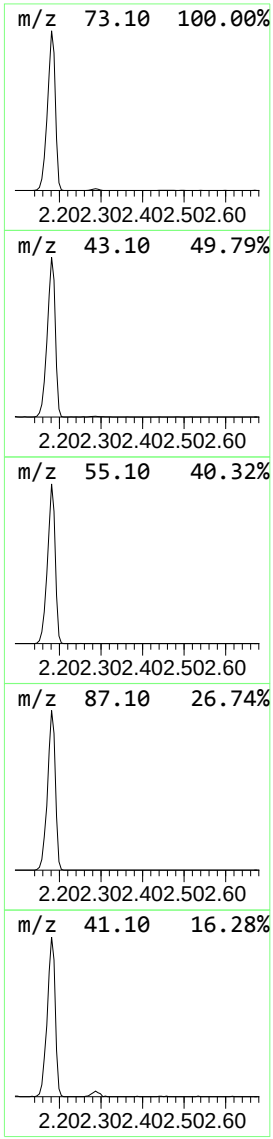
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	200.54 ng	2840400	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	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9





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Data File : BF123959.D
Acq On : 17 May 2021 12:56
Operator : JU/CG
Sample : M2322-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3-20210505

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

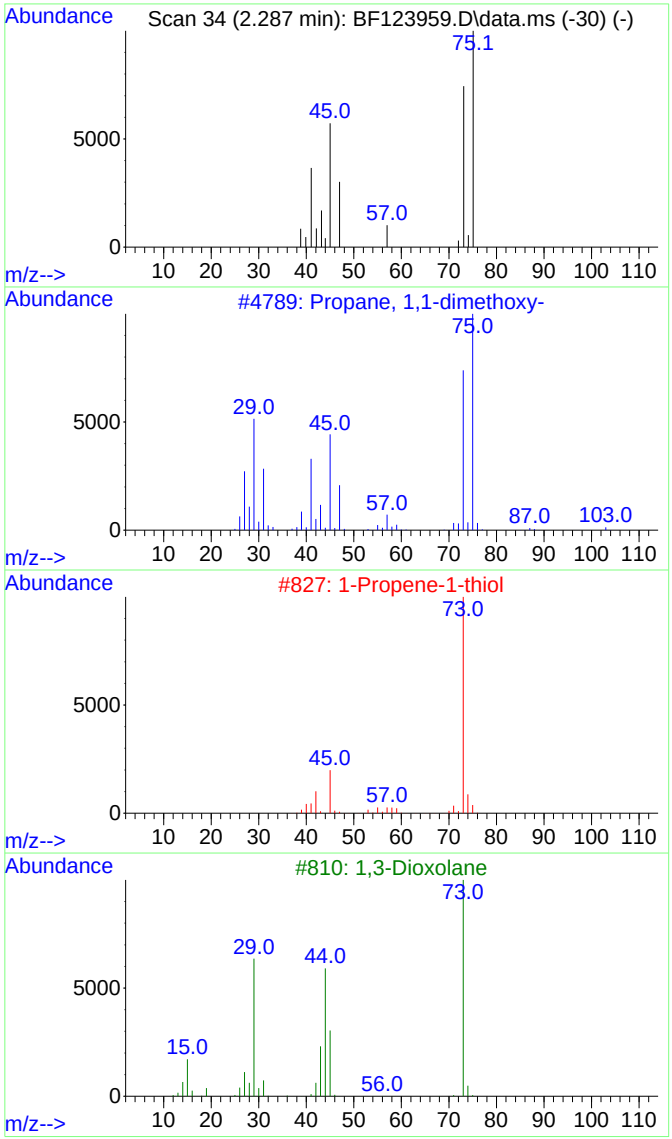
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

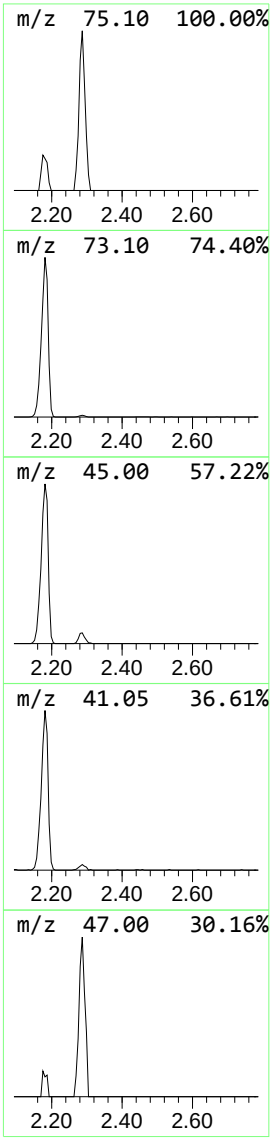
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	3.24 ng	45892	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2	1-Propene-1-thiol	74	C3H6S	000925-89-3	7
3	1,3-Dioxolane	74	C3H6O2	000646-06-0	7
4	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	4
5	Glycine	75	C2H5NO2	000056-40-6	4





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Acq On : 17 May 2021 12:56
Operator : JU/CG
Sample : M2322-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3-20210505

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

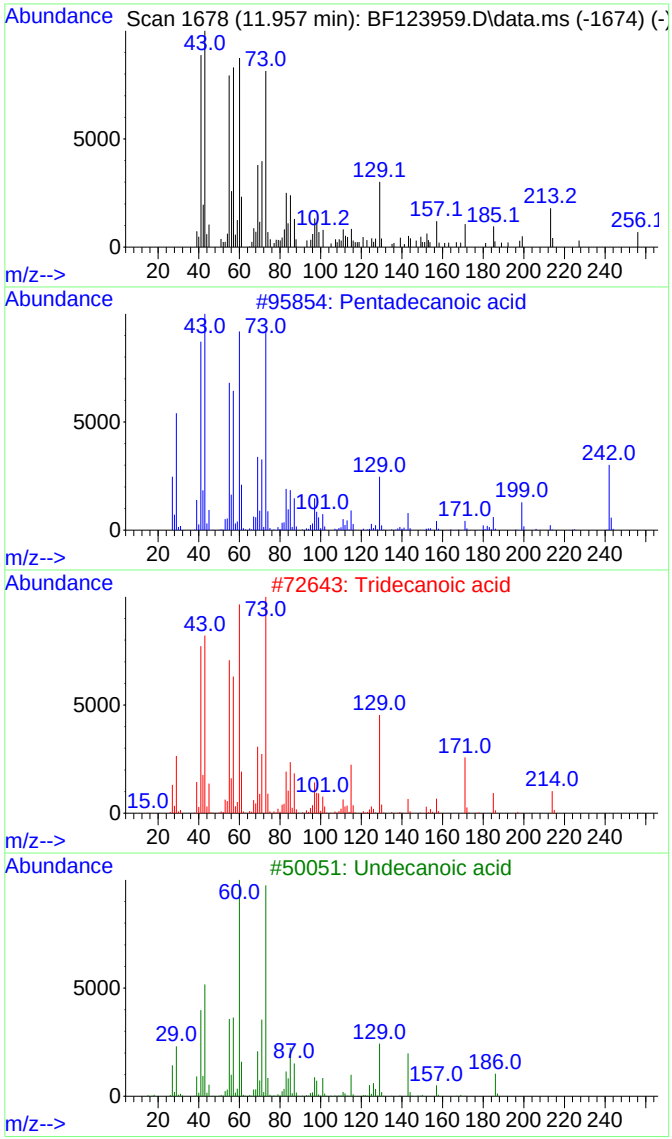
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

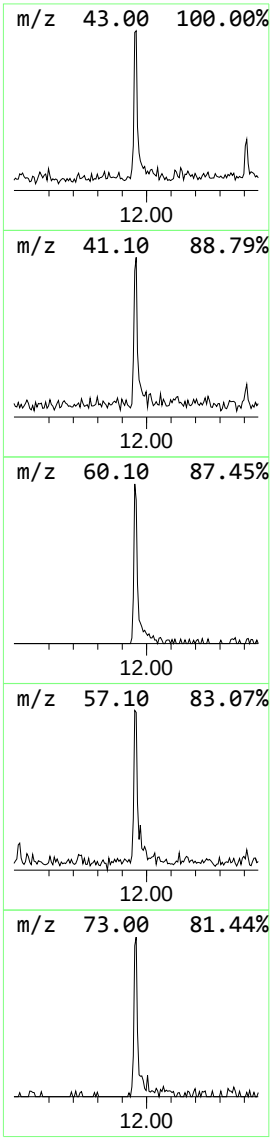
****

Peak Number 3 Pentadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	9.39 ng	225016	Phenanthrene-d10	11.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
2	Tridecanoic acid	214	C13H26O2	000638-53-9	81
3	Undecanoic acid	186	C11H22O2	000112-37-8	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	43





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Acq On : 17 May 2021 12:56
Operator : JU/CG
Sample : M2322-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3-20210505

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

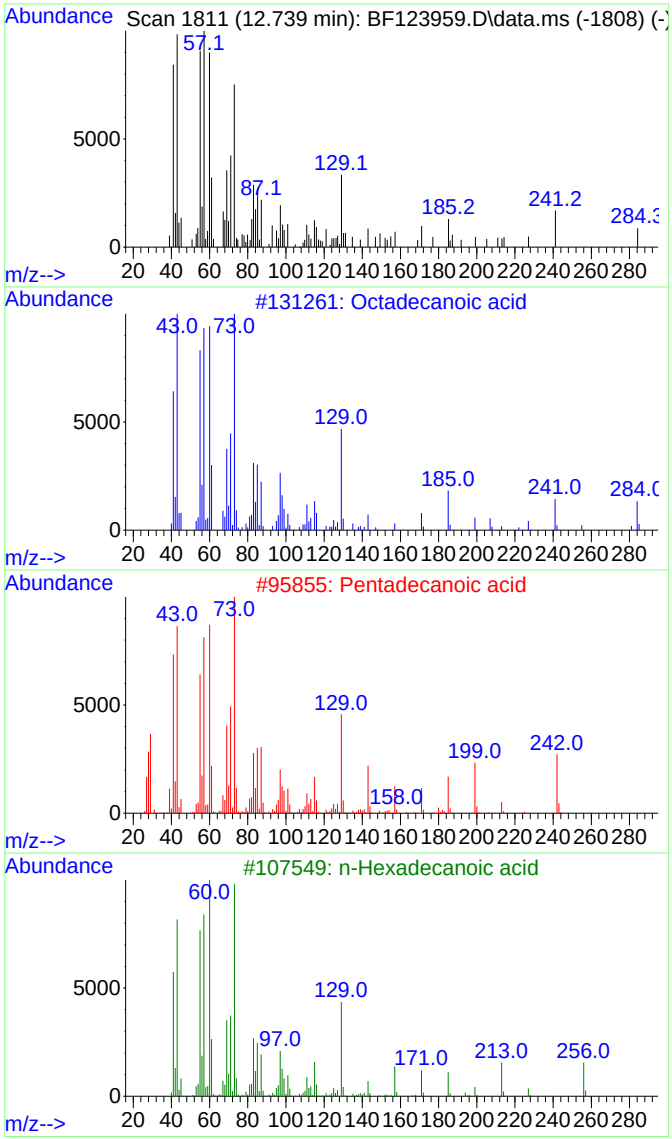
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

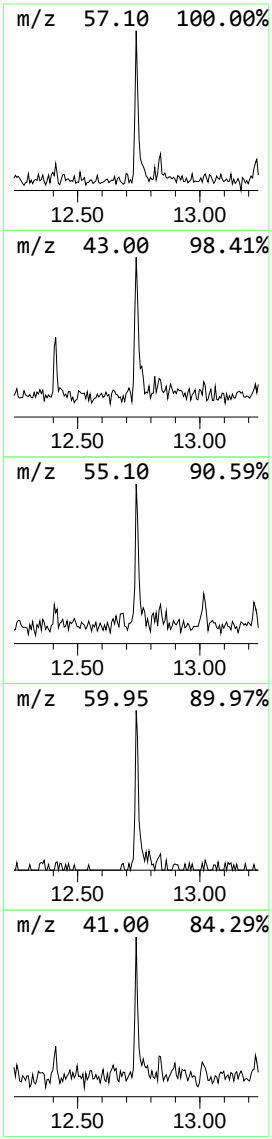
****

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.739	5.21 ng	124775	Phenanthrene-d10	11.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	38
5	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123959.D
Acq On : 17 May 2021 12:56
Operator : JU/CG
Sample : M2322-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3-20210505

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

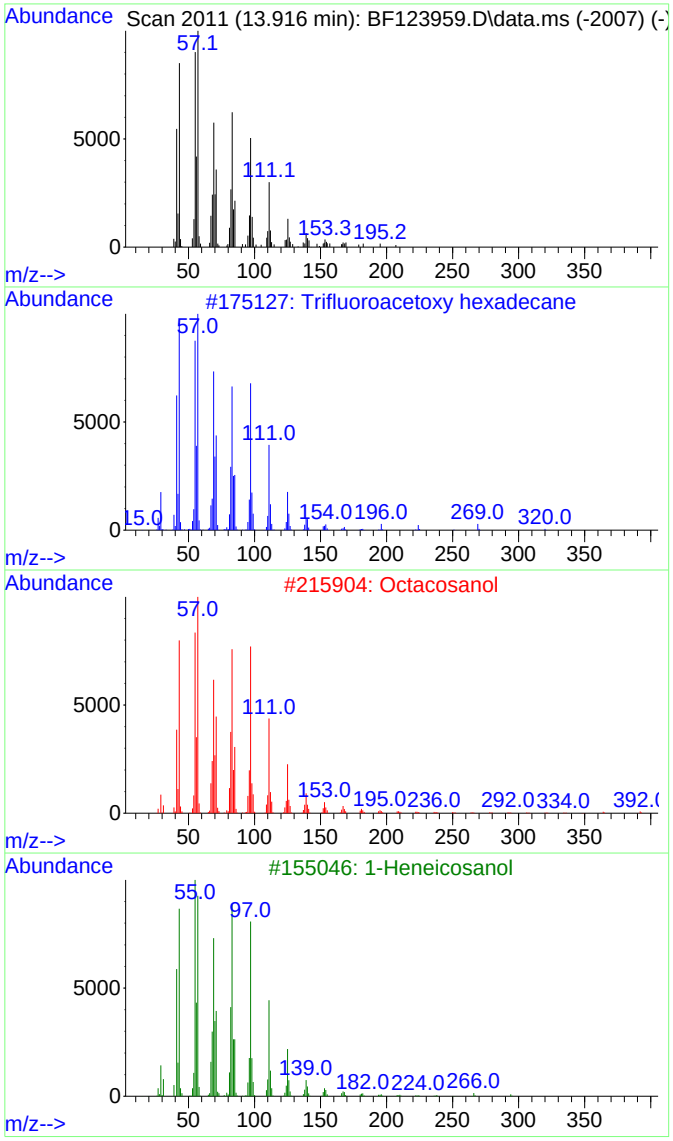
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

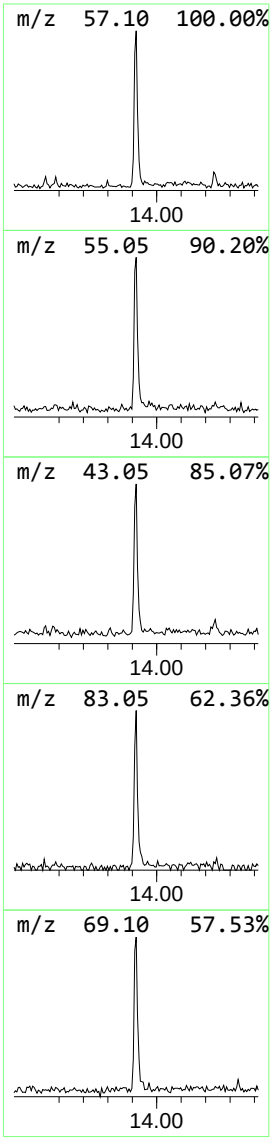
****

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	12.09 ng	248572	Chrysene-d12	14.069

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2	Octacosanol	410	C28H58O	000557-61-9	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





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Operator : JU/CG
Sample : M2322-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3-20210505

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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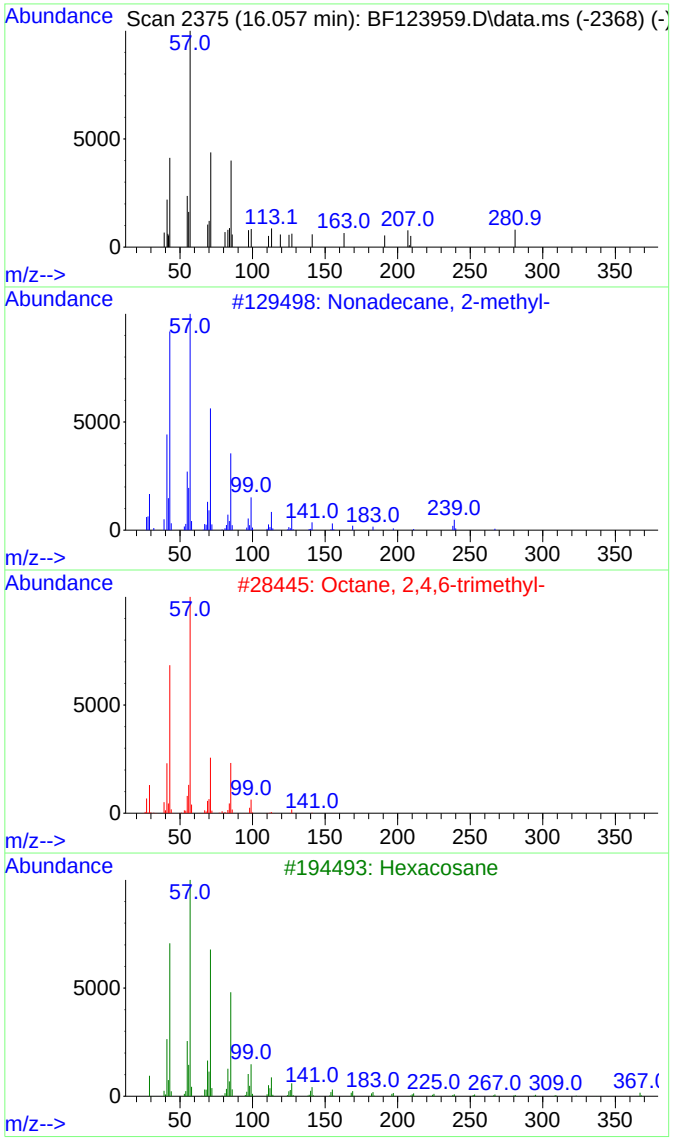
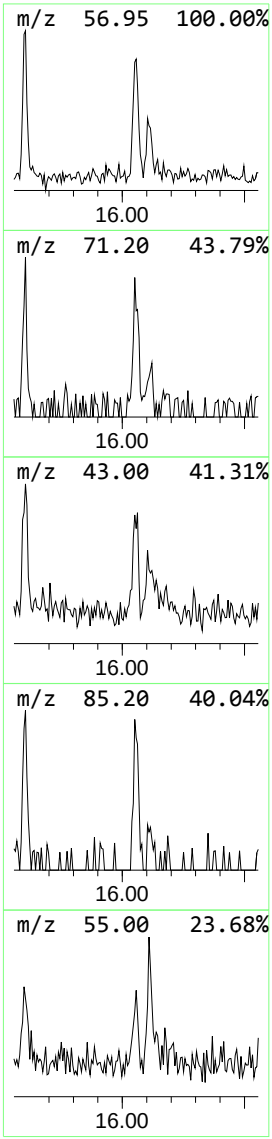
****
Peak Number 6 Nonadecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.057	2.30 ng	39209	Perylene-d12	15.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	64
2	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	59
3	Hexacosane	366	C26H54	000630-01-3	58
4	Nonadecane	268	C19H40	000629-92-5	53
5	Pentadecane	212	C15H32	000629-62-9	53





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Data File : BF123959.D
Acq On : 17 May 2021 12:56
Operator : JU/CG
Sample : M2322-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3-20210505

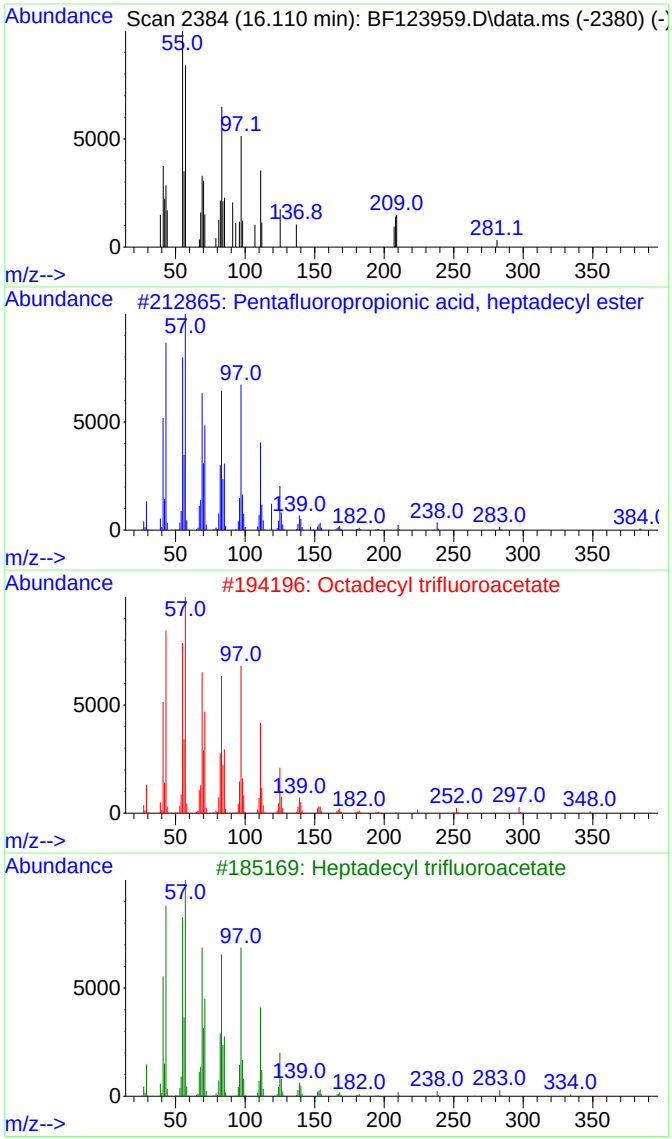
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

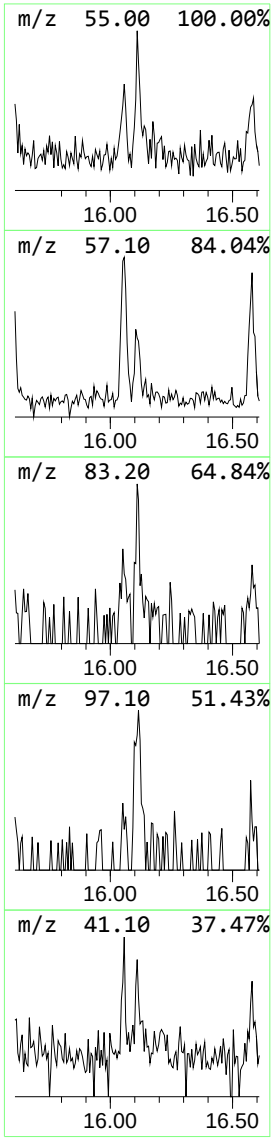
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.110	2.14 ng	36594	Perylene-d12	15.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	76
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	76
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	76
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	68
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	68





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TIC Library : C:\DATABASE\NIST11.L
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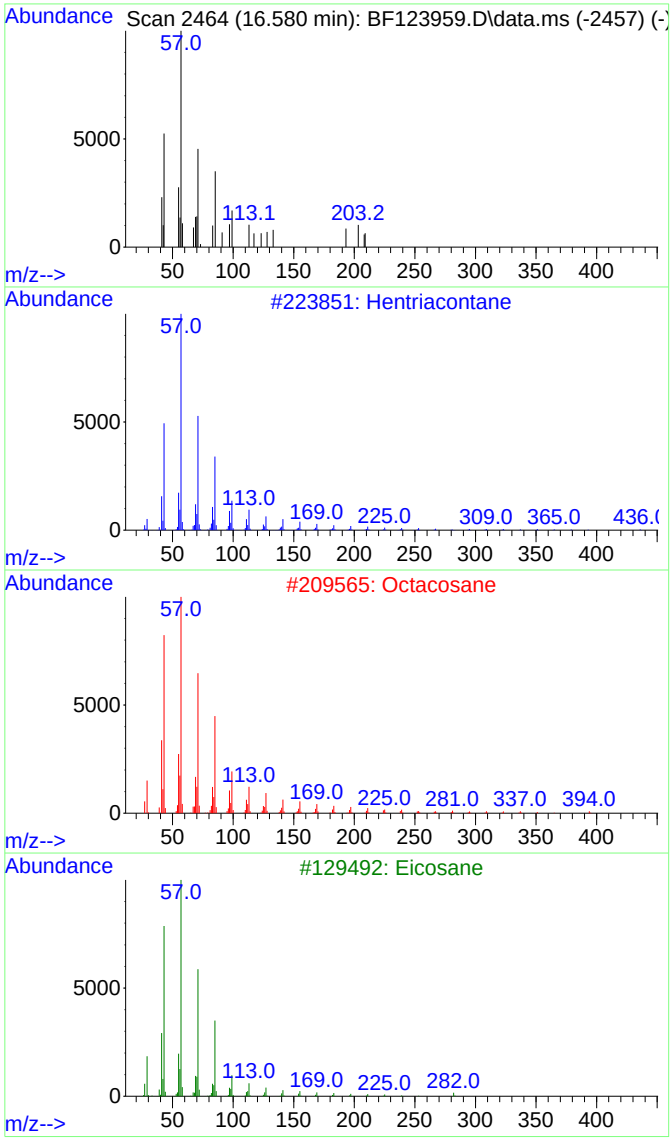
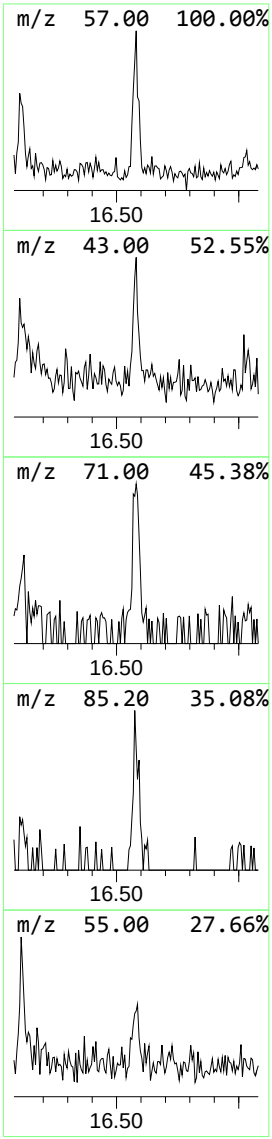
Peak Number 8 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.580	2.32 ng	39581	Perylene-d12	15.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	64
2	Octacosane	394	C28H58	000630-02-4	64
3	Eicosane	282	C20H42	000112-95-8	59
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	59
5	Heneicosane	296	C21H44	000629-94-7	59





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Data File : BF123959.D
Acq On : 17 May 2021 12:56
Operator : JU/CG
Sample : M2322-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3-20210505

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

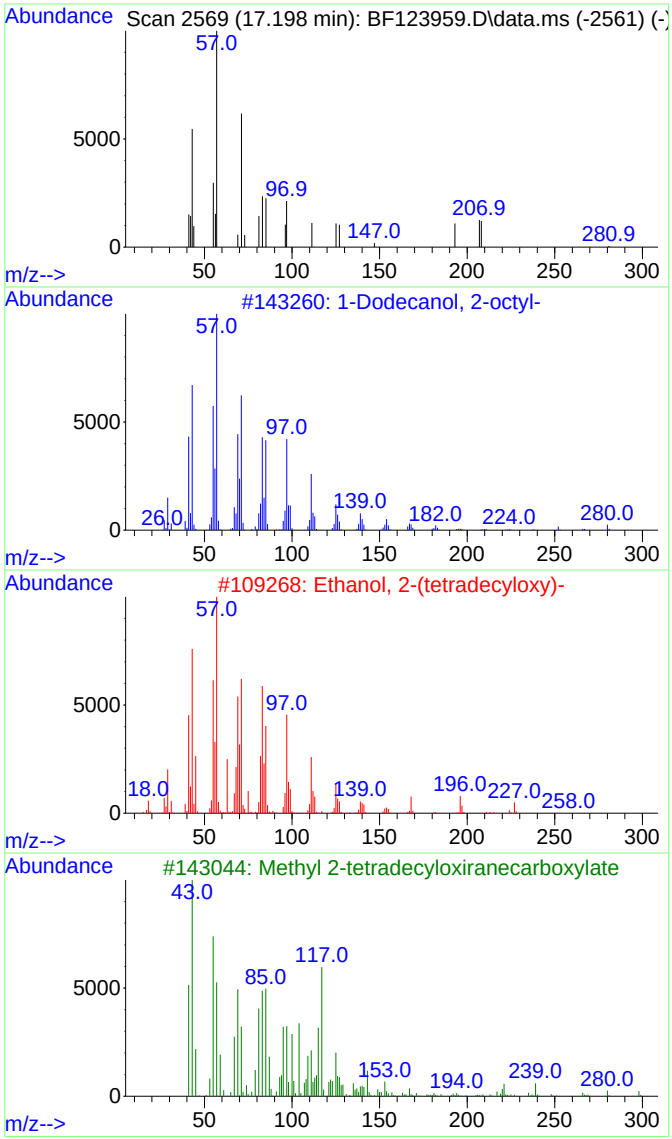
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

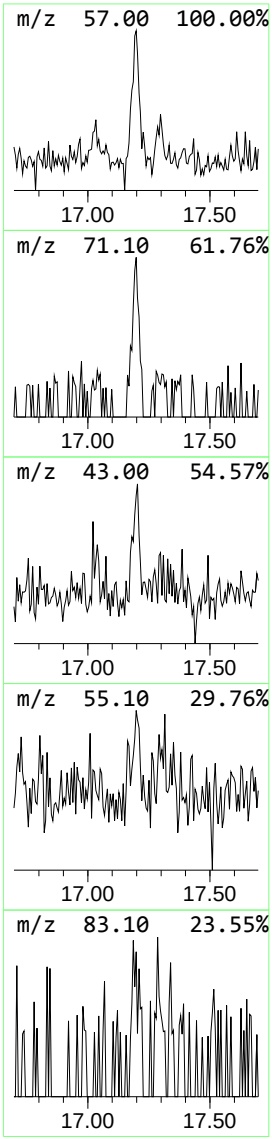
****

Peak Number 9 unknown17.19 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.198	2.08 ng	35504	Perylene-d12	15.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	43
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	43
3	Methyl 2-tetradecyloxiranecarbox...	298	C18H34O3	1000213-09-0	35
4	17-Pentatriacontene	491	C35H70	006971-40-0	35
5	Triacontyl acetate	480	C32H64O2	041755-58-2	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051721\
Data File : BF123959.D
Acq On : 17 May 2021 12:56
Operator : JU/CG
Sample : M2322-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-3-20210505

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.181	200.5	ng	2840400	1	6.904	283276	20.0
Propane, 1,1-di...	2.287	3.2	ng	45892	1	6.904	283276	20.0
Pentadecanoic acid	11.957	9.4	ng	225016	4	11.428	479225	20.0
Octadecanoic acid	12.739	5.2	ng	124775	4	11.428	479225	20.0
Trifluoroacetox...	13.916	12.1	ng	248572	5	14.069	411188	20.0
Nonadecane, 2-m...	16.057	2.3	ng	39209	6	15.563	341303	20.0
Pentafluoroprop...	16.110	2.1	ng	36594	6	15.563	341303	20.0
Hentriacontane	16.580	2.3	ng	39581	6	15.563	341303	20.0
unknown17.19	17.198	2.1	ng	35504	6	15.563	341303	20.0