LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042121\
Data File : BF123663.D
Acq On : 21 Apr 2021 12:56
Operator : JU/CG
Sample : M2076-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-0-2.0

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-BF041521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123663.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	496	506	510	rBV	41482	61315	1.17%	0.145%
2	5.469	572	575	588	rVB	5306238	5053117	96.83%	11.946%
3	6.486	743	748	759	rBV	5250860	5218712	100.00%	12.337%
4	6.851	806	810	813	rBV	1573123	1310772	25.12%	3.099%
5	7.410	900	905	908	rBV	3922590	3399789	65.15%	8.037%
6	8.133	1024	1028	1031	rBV	2157782	1652304	31.66%	3.906%
7	9.210	1207	1211	1215	rBV	5305340	4890783	93.72%	11.562%
8	9.604	1275	1278	1282	rBV	163251	134352	2.57%	0.318%
9	9.892	1323	1327	1330	rBV	2196689	1720532	32.97%	4.067%
10	10.098	1358	1362	1370	rBV3	76761	102278	1.96%	0.242%
11	10.680	1457	1461	1465	rBV	3491698	3234783	61.98%	7.647%
12	11.380	1576	1580	1584	rBV	2156126	1813421	34.75%	4.287%
13	11.916	1663	1671	1680	rBV	545394	708961	13.58%	1.676%
14	12.304	1733	1737	1741	rBV	226478	209898	4.02%	0.496%
15	12.474	1759	1766	1769	rBV8	30954	72092	1.38%	0.170%
16	12.704	1800	1805	1817	rBV	879907	1124888	21.55%	2.659%
17	12.798	1817	1821	1823	rVV3	63888	78270	1.50%	0.185%
18	12.974	1846	1851	1854	rBV	5412558	4716870	90.38%	11.151%
19	13.157	1879	1882	1888	rVB4	63016	73450	1.41%	0.174%
20	13.351	1910	1915	1923	rVB4	97565	222364	4.26%	0.526%
21	13.445	1927	1931	1938	rVB3	99336	132493	2.54%	0.313%
22	13.527	1938	1945	1947	rBV3	179156	239224	4.58%	0.566%
23	13.892	1999	2007	2010	rBV3	157920	319489	6.12%	0.755%
24	13.933	2010	2014	2025	rVV2	282393	726816	13.93%	1.718%
25	14.027	2026	2030	2034	rVB	1738762	1498090	28.71%	3.542%
26	14.151	2046	2051	2055	rVB2	91118	147351	2.82%	0.348%
27	14.198	2056	2059	2061	rBV	112153	107106	2.05%	0.253%
28	14.504	2107	2111	2115	rVB	182011	172150	3.30%	0.407%
29	14.768	2151	2156	2160	rBV3	78814	148216	2.84%	0.350%
30	14.815	2160	2164	2169	rVB	192020	219257	4.20%	0.518%
31	14.962	2186	2189	2192	rVB	67319	64749	1.24%	0.153%
32	15.156	2218	2222	2228	rBV	277755	333227	6.39%	0.788%
33	15.509	2277	2282	2285	rBV	890098	1137534	21.80%	2.689%
34	15.545	2285	2288	2296	rVB	212903	279613	5.36%	0.661%
35	15.751	2320	2323	2327	rVB5	42680	54988	1.05%	0.130%
36	15.992	2359	2364	2369	rVB	212350	335648	6.43%	0.793%

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Integrator: RTE
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Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	16.503	2447	2451	2456	rVV3	87481	142735	2.74%	0.337%
38	16.586	2459	2465	2474	rVB4	110284	288329	5.52%	0.682%
39	17.115	2549	2555	2561	rVB4	66177	154994	2.97%	0.366%

Sum of corrected areas: 42300960

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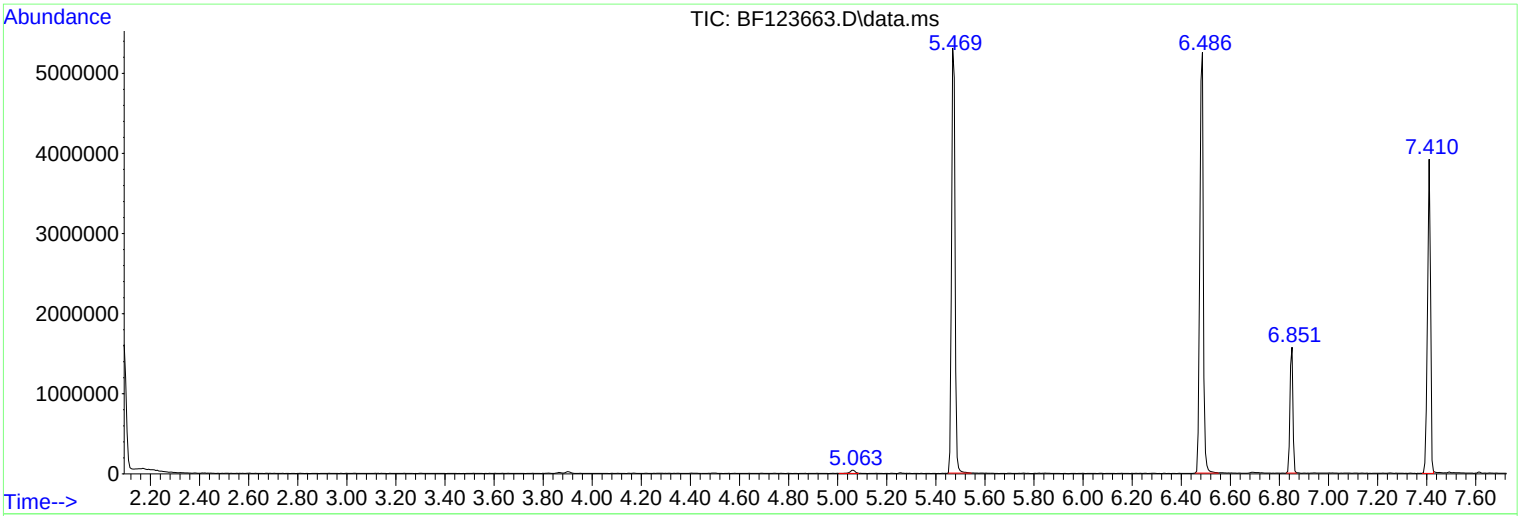
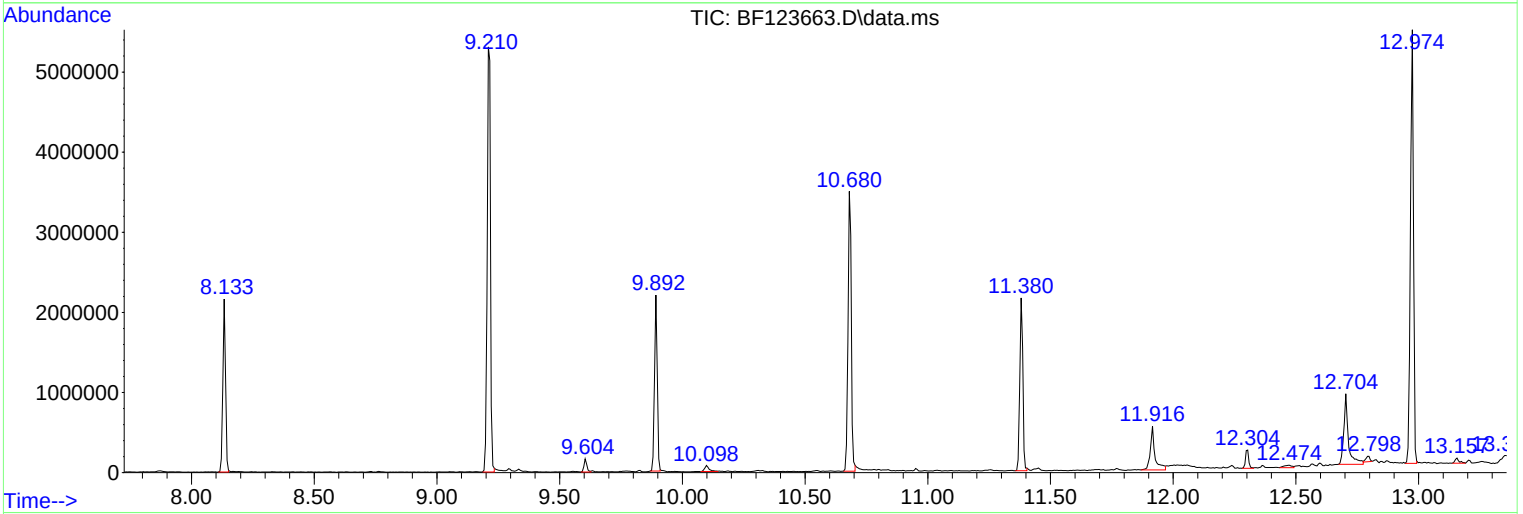
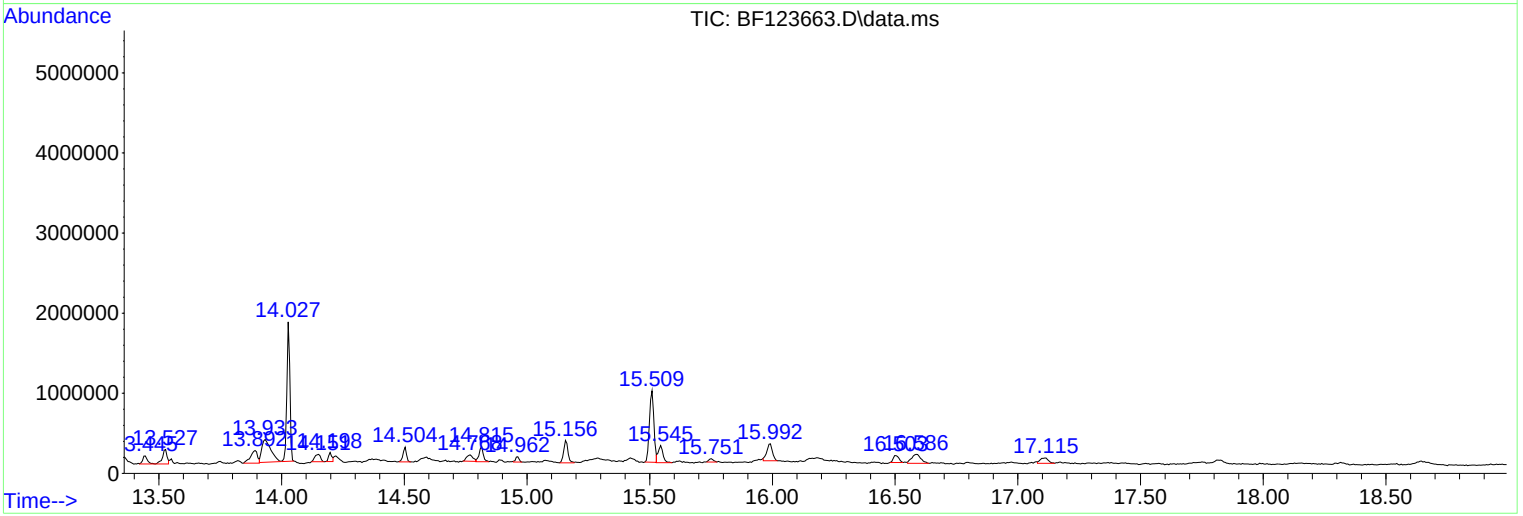
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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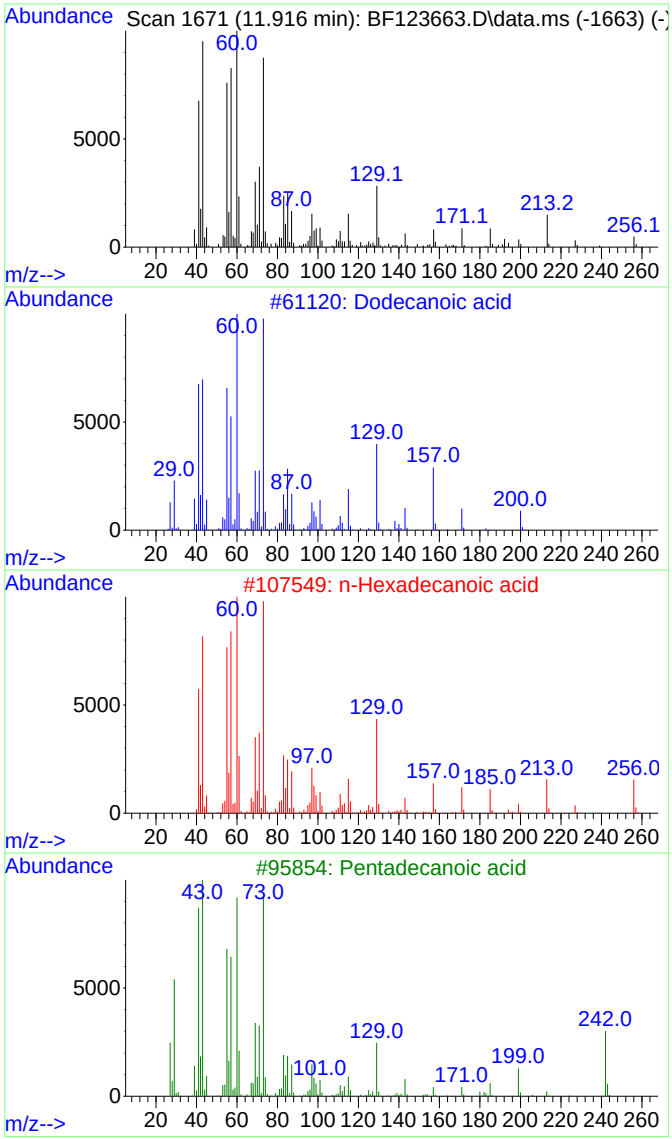
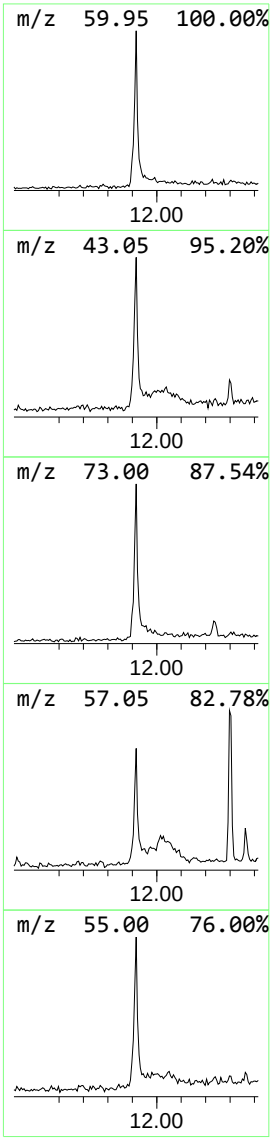
Peak Number 1 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	7.82 ng	708961	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	91
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	80





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Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
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TIC Library : C:\DATABASE\NIST11.L
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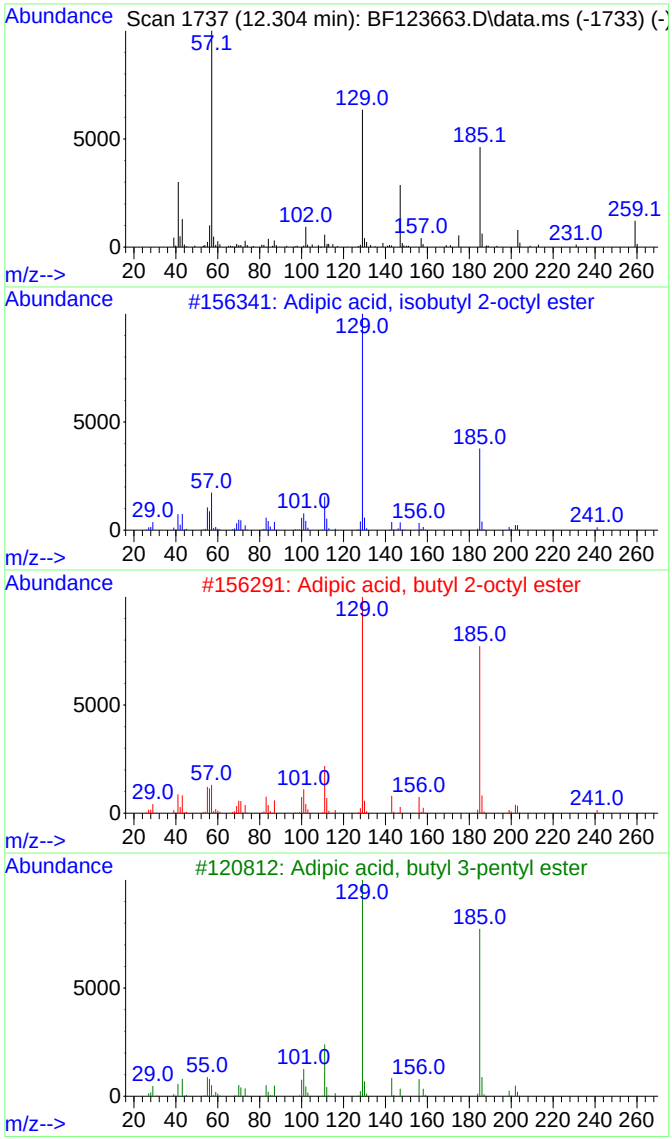
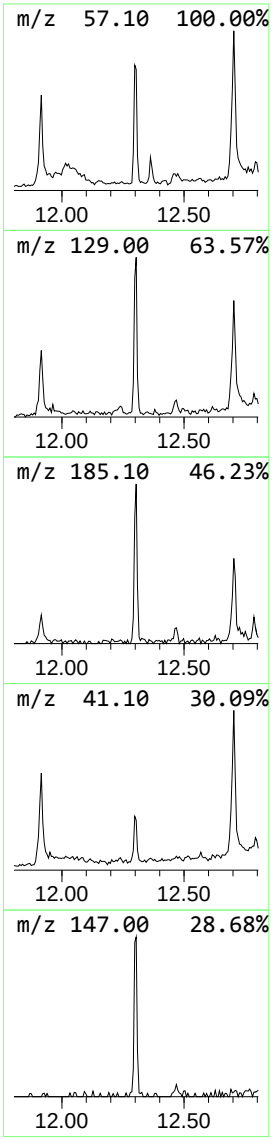
Peak Number 2 unknown12.30 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.304	2.31 ng	209898	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	45
2	Adipic acid, butyl 2-octyl ester	314	C18H34O4	1000324-44-6	38
3	Adipic acid, butyl 3-pentyl ester	272	C15H28O4	1000324-60-5	37
4	Adipic acid, butyl 3-heptyl ester	300	C17H32O4	1000353-64-9	37
5	Adipic acid, butyl 2-hexyl ester	286	C16H30O4	1000353-71-0	37





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Instrument : BNA_F
ClientSampleId : SB-17-0-2.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.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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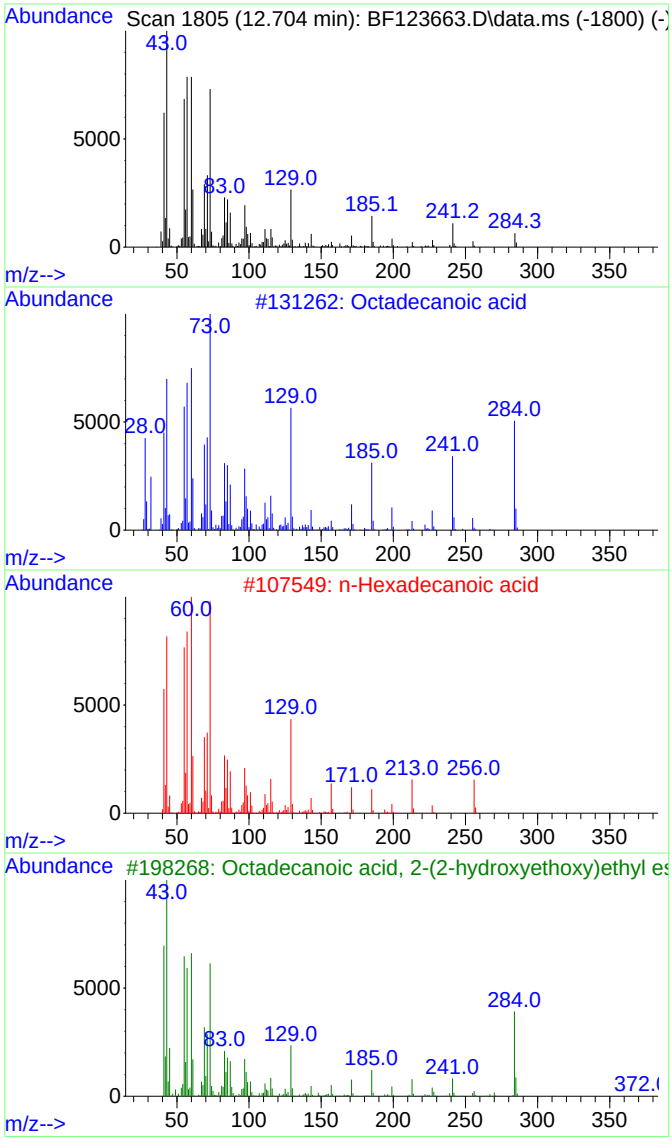
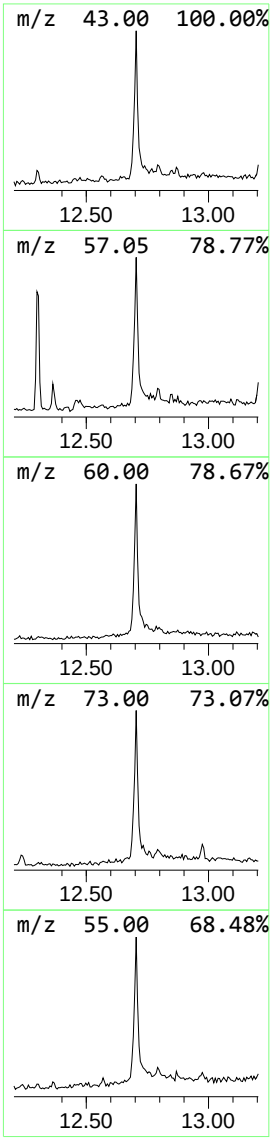
Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	12.41 ng	1124890	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	58





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
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TIC Library : C:\DATABASE\NIST11.L
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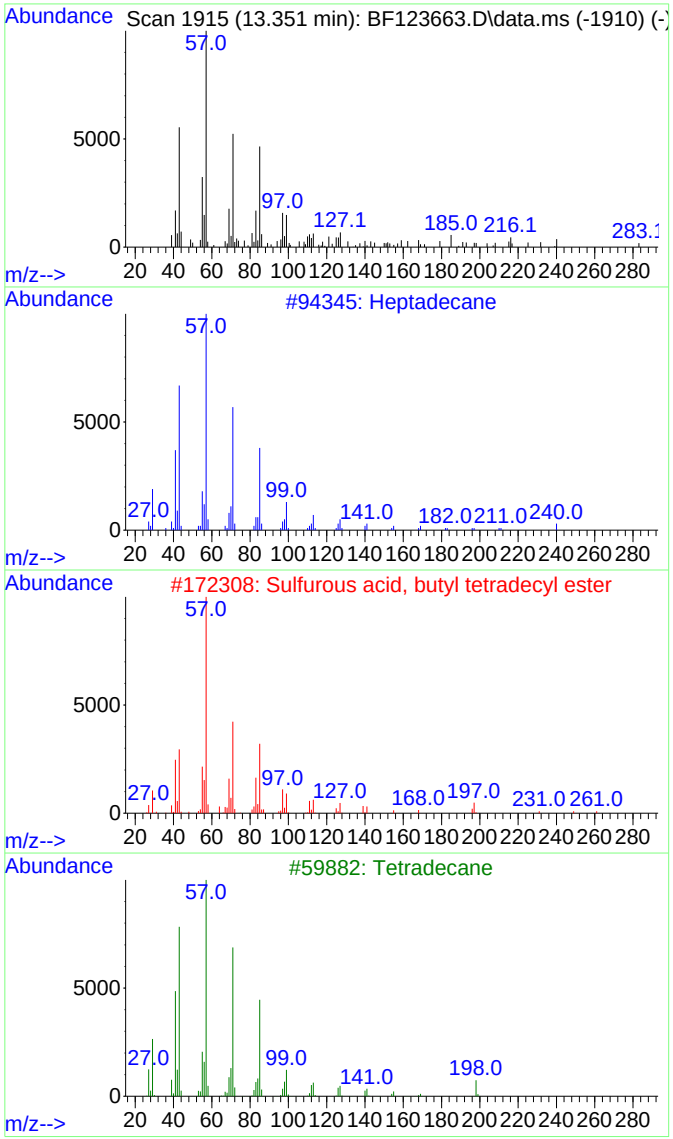
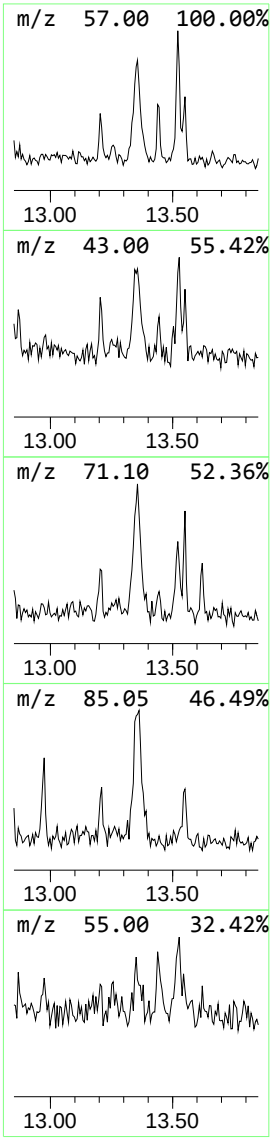
Peak Number 4 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.351	2.97 ng	222364	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	83
2	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	80
3	Tetradecane	198	C14H30	000629-59-4	74
4	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	72
5	Octadecane	254	C18H38	000593-45-3	64





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Misc :
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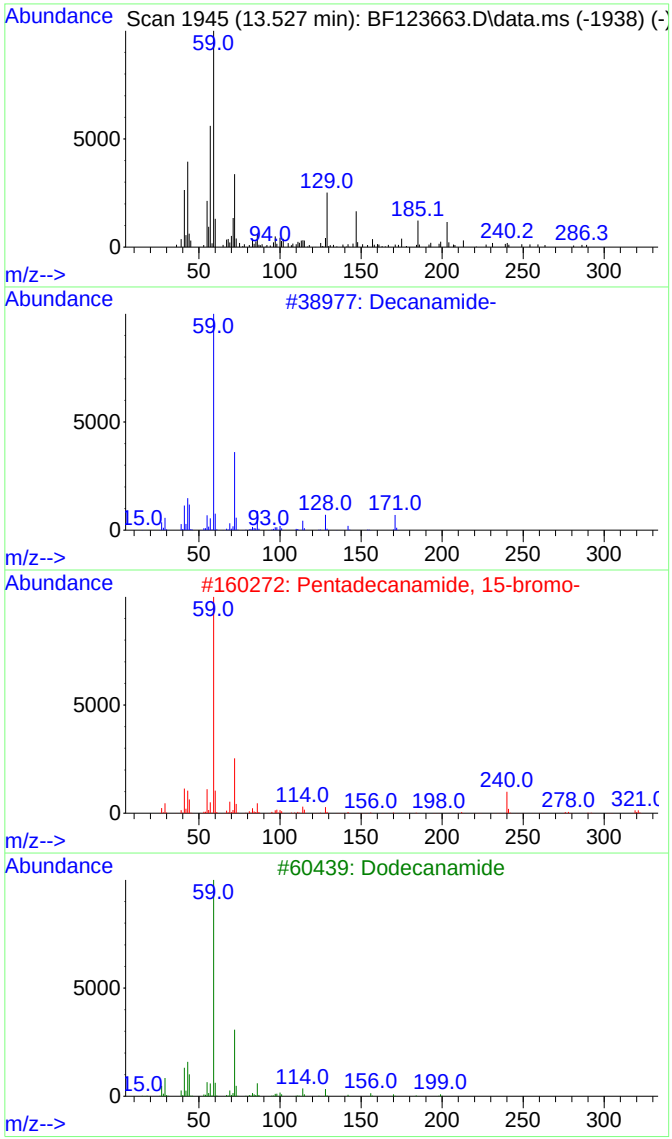
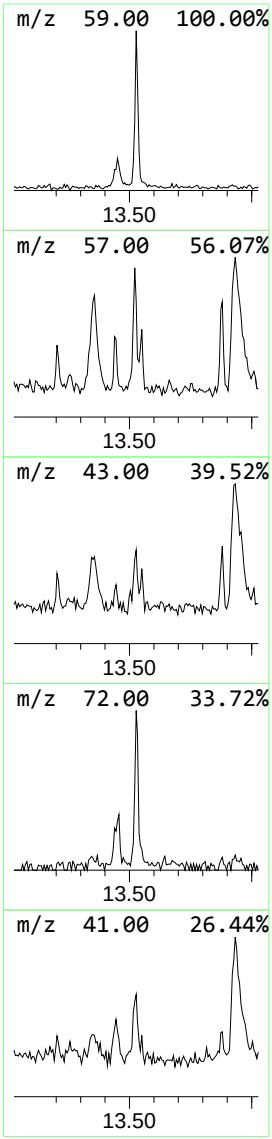
Peak Number 5 Decanamide- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.527	3.19 ng	239224	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanamide-	171	C10H21NO	002319-29-1	50
2	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	50
3	Dodecanamide	199	C12H25NO	001120-16-7	47
4	Nonadecanamide	297	C19H39NO	058185-32-3	40
5	Hexadecanamide	255	C16H33NO	000629-54-9	40





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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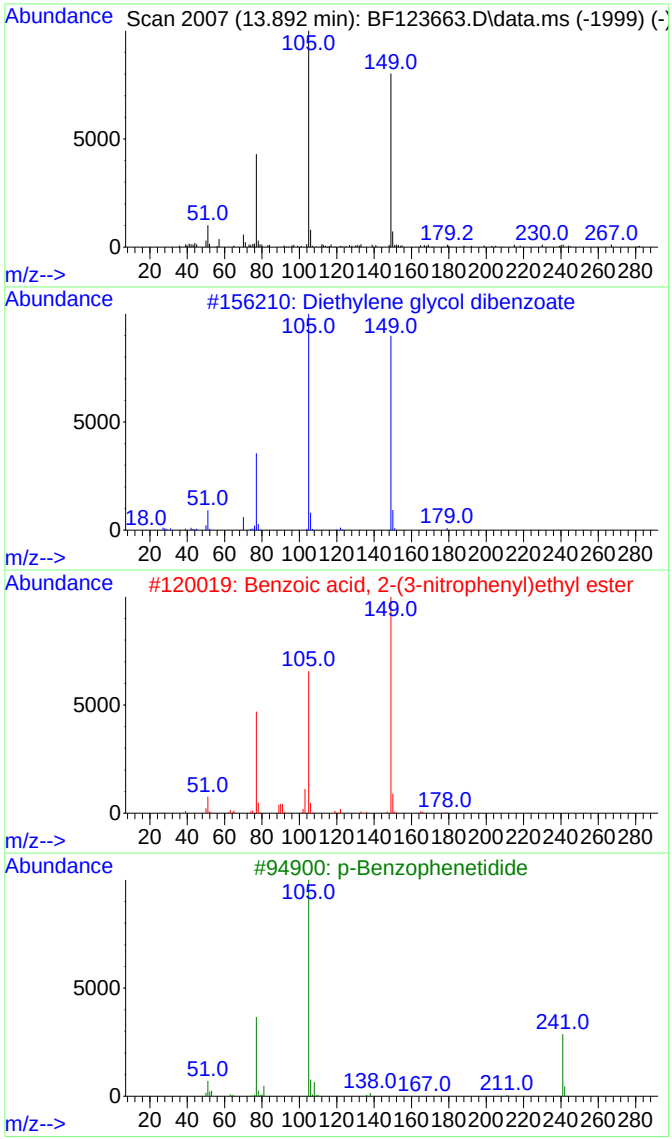
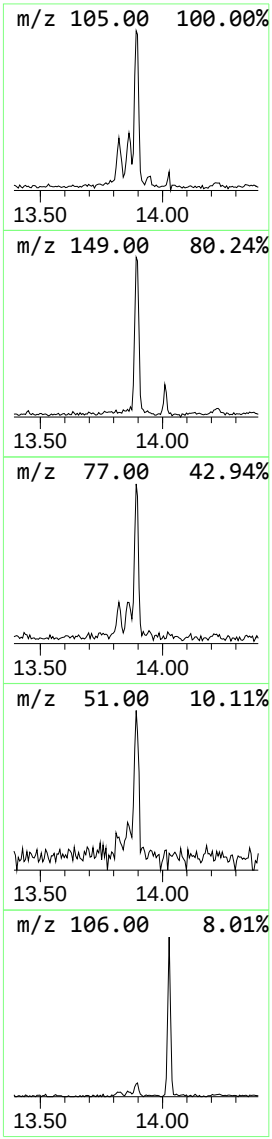
Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	4.27 ng	319489	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
2	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
3	p-Benzophenetidide	241	C15H15NO2	015437-14-6	38
4	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	35
5	2,5-Cyclohexadiene-1,4-dione, 5-...	289	C15H12ClNO3	324051-60-7	35





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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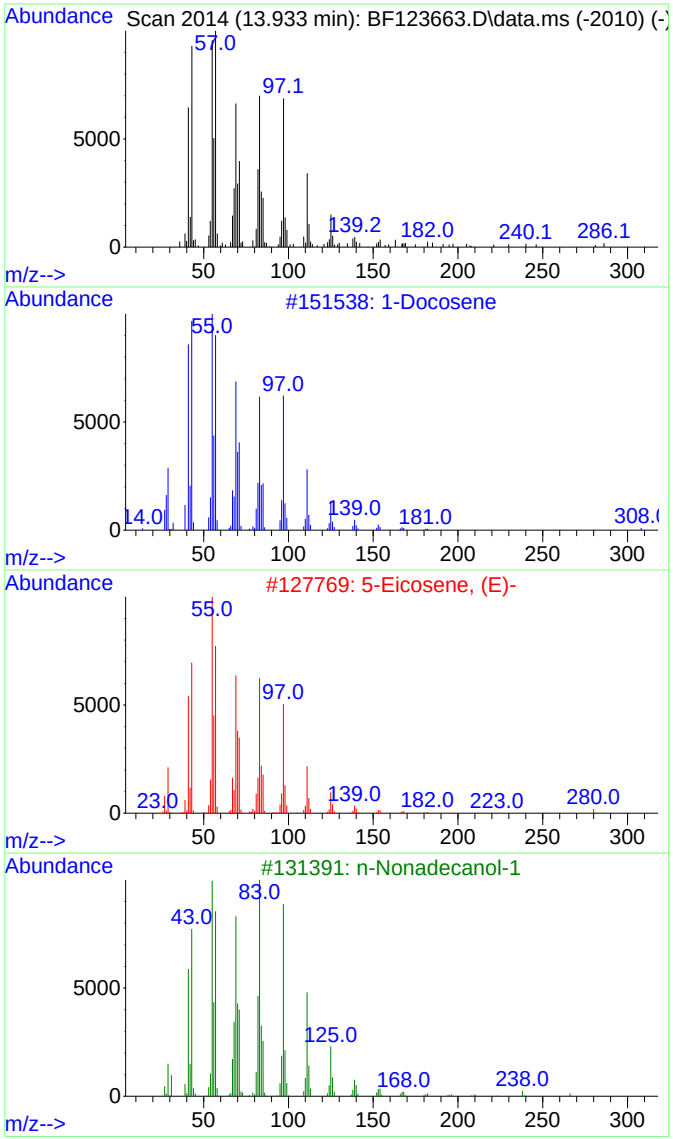
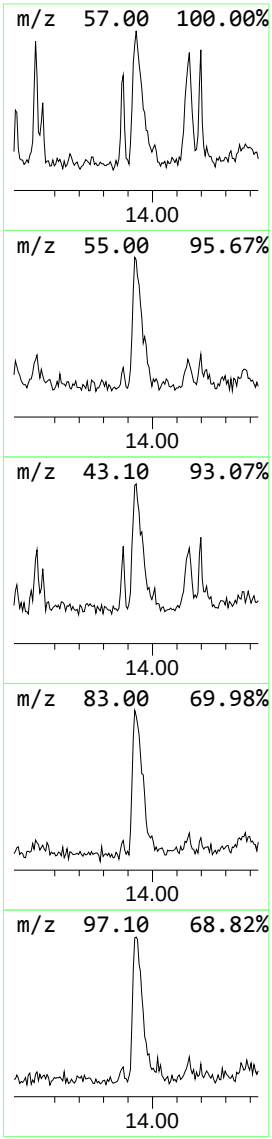
Peak Number 7 1-Docosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	9.70 ng	726816	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
5	1-Heneicosanol	312	C21H44O	015594-90-8	90





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Sample : M2076-13
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Instrument :
BNA_F
ClientSampleId :
SB-17-0-2.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.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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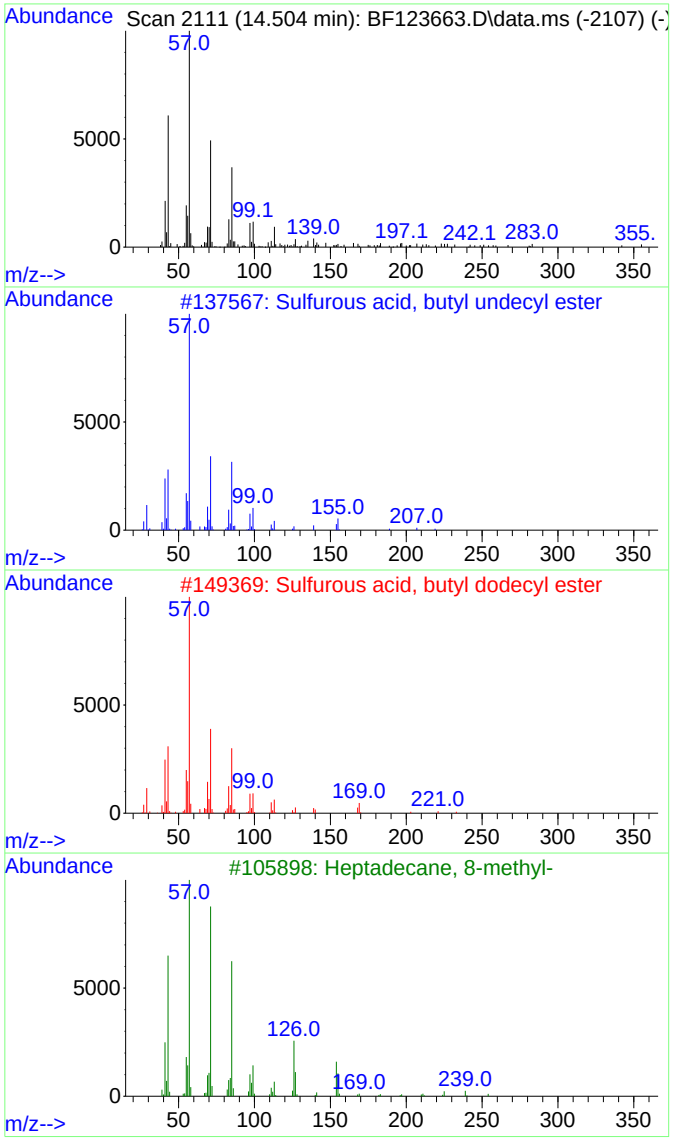
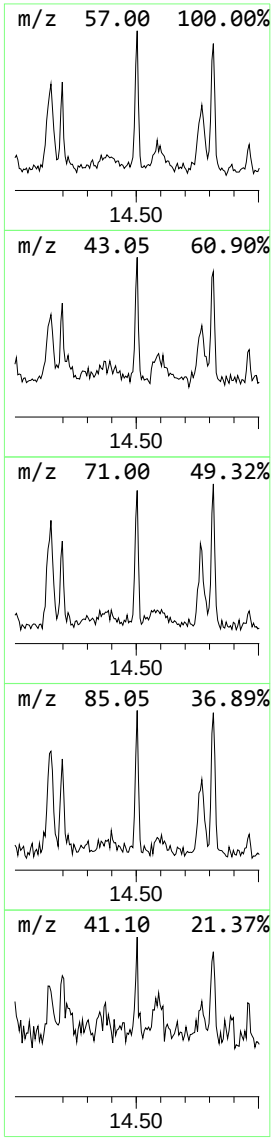
Peak Number 8 Sulfurous acid, butyl undec... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	2.30 ng	172150	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	87
2	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	86
3	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	72
4	Sulfurous acid, butyl decyl ester	278	C14H30O3S	1000309-17-7	72
5	Octacosane	394	C28H58	000630-02-4	64





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Acq On : 21 Apr 2021 12:56
Operator : JU/CG
Sample : M2076-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-17-0-2.0

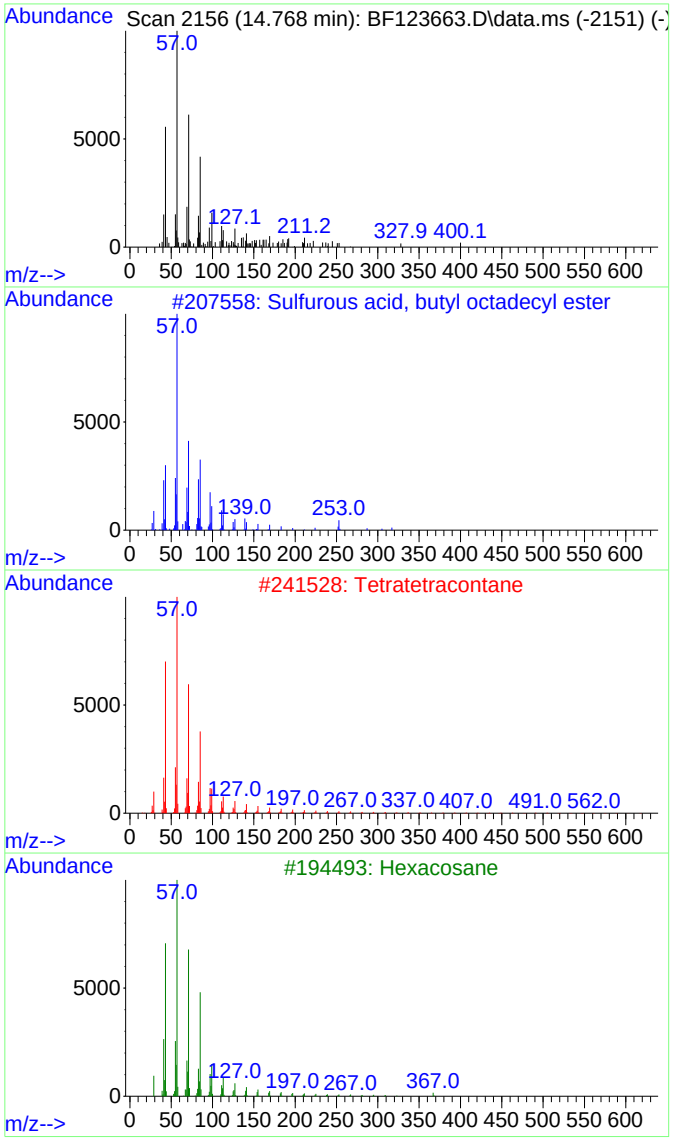
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

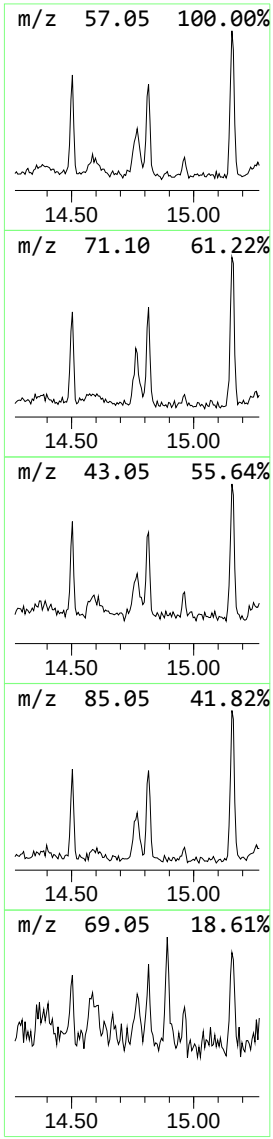
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Sulfurous acid, butyl octad... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.768	2.61 ng	148216	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	72
2	Tetratetracontane	619	C44H90	007098-22-8	72
3	Hexacosane	366	C26H54	000630-01-3	72
4	Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	72
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	72





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Sample : M2076-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-0-2.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.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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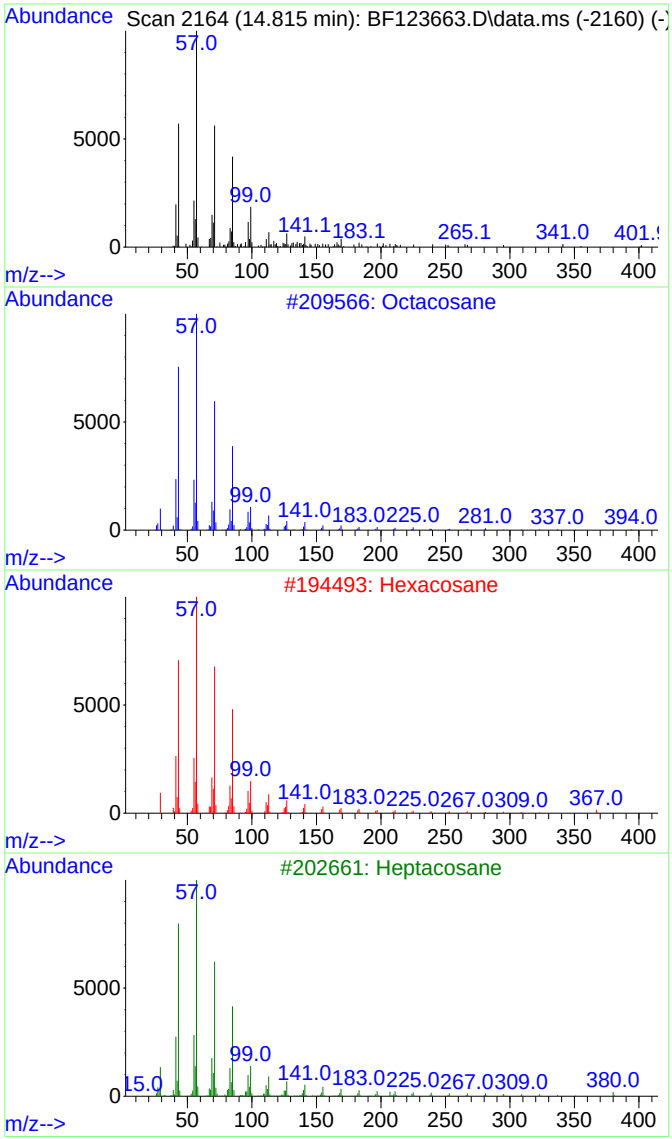
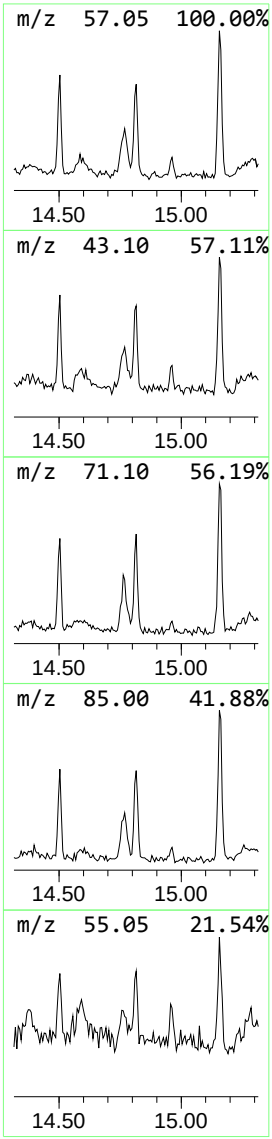
Peak Number 10 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.815	3.85 ng	219257	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heptacosane	380	C27H56	000593-49-7	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Tetratetracontane	619	C44H90	007098-22-8	87





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Operator : JU/CG
Sample : M2076-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-0-2.0

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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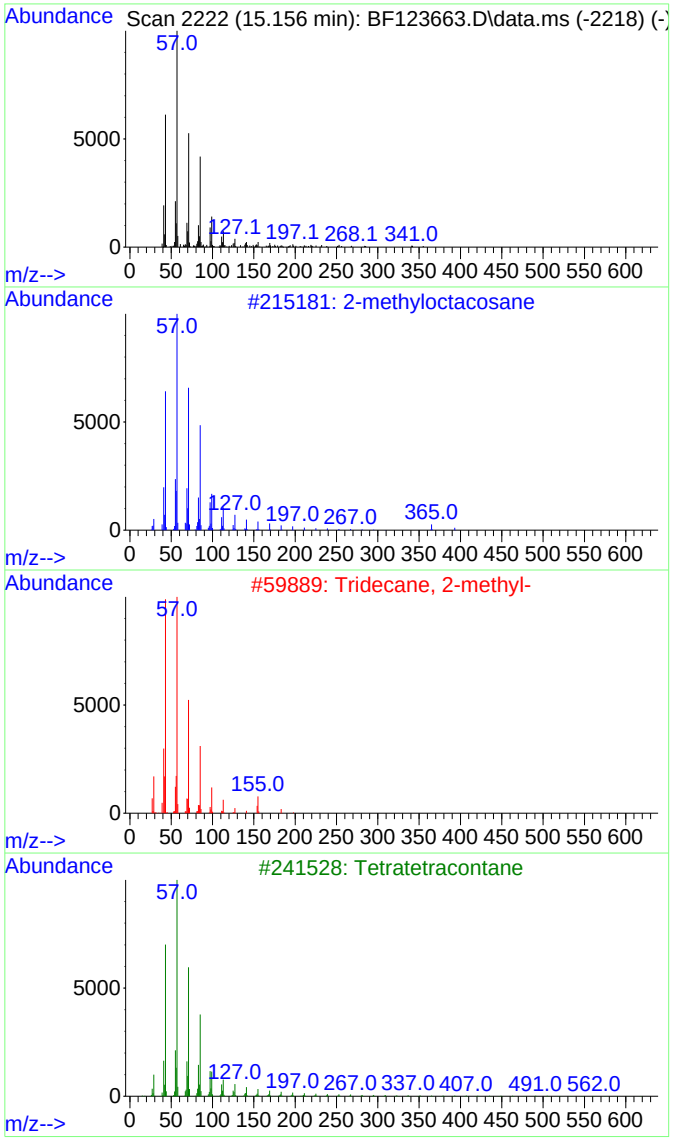
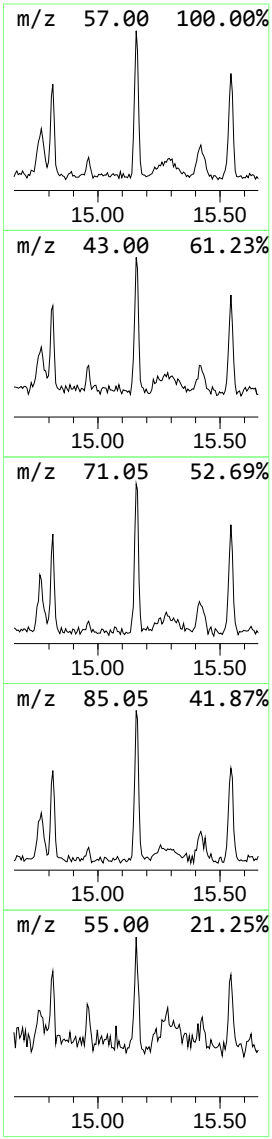
Peak Number 11 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.156	5.86 ng	333227	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	86
2	Tridecane, 2-methyl-	198	C14H30	001560-96-9	83
3	Tetratetracontane	619	C44H90	007098-22-8	74
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	72
5	Heptacosane	380	C27H56	000593-49-7	68





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Operator : JU/CG
Sample : M2076-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-17-0-2.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.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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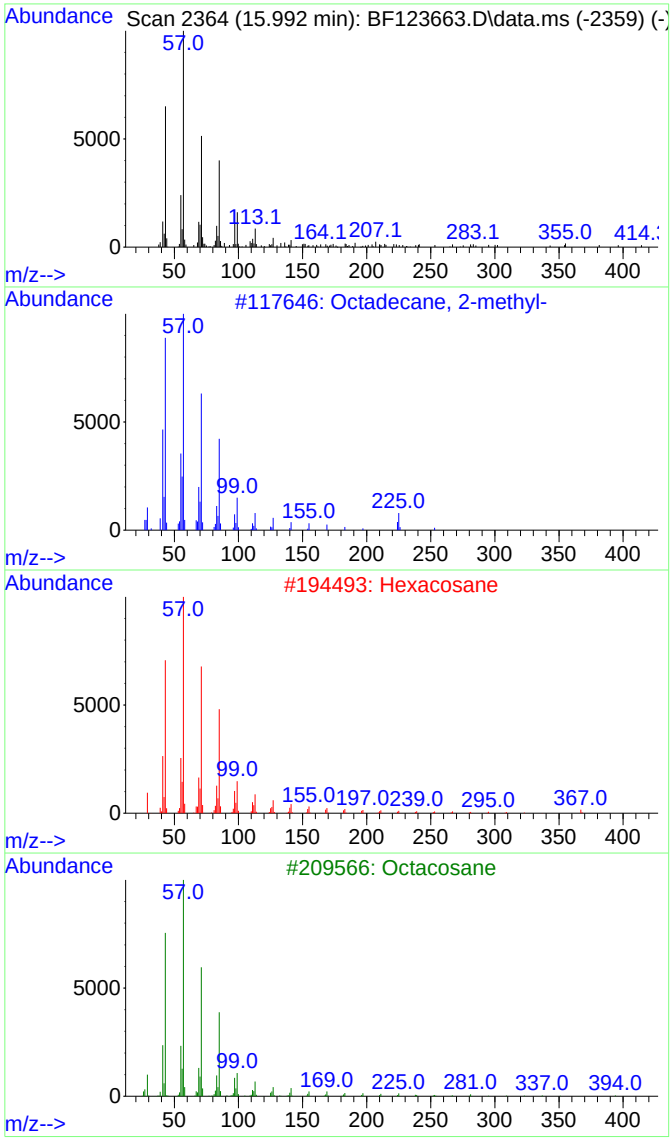
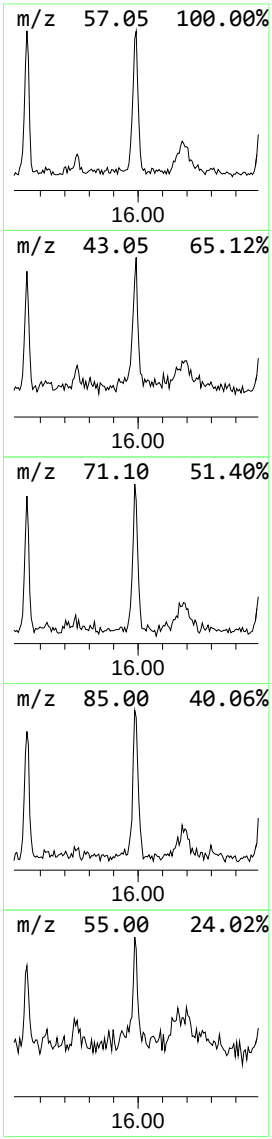
Peak Number 12 Octadecane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.992	5.90 ng	335648	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	87
2	Hexacosane	366	C26H54	000630-01-3	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Pentacosane	352	C25H52	000629-99-2	86
5	Eicosane	282	C20H42	000112-95-8	80





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Operator : JU/CG
Sample : M2076-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-17-0-2.0

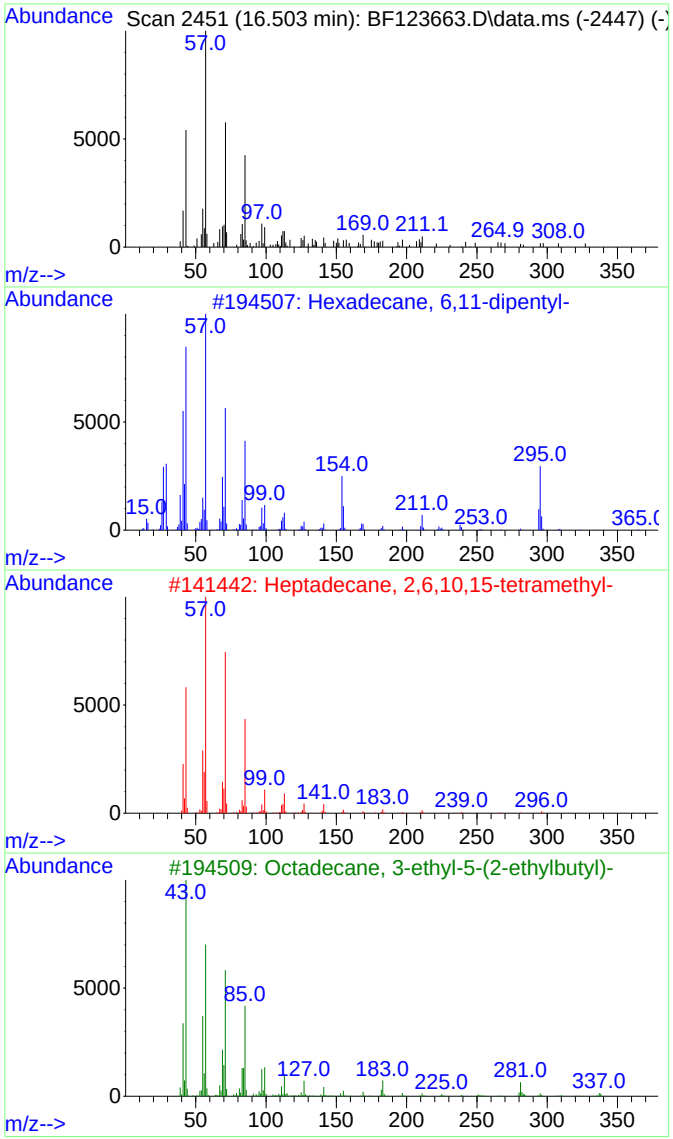
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

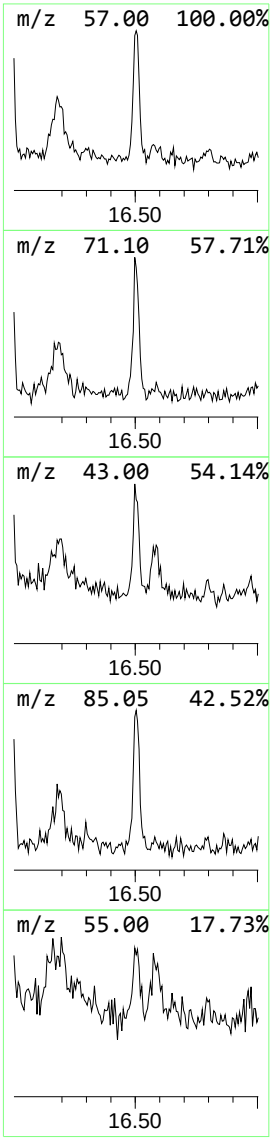
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Hexadecane, 6,11-dipentyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.503	2.51 ng	142735	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 6,11-dipentyl-	366	C26H54	015874-03-0	78
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	72
3	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	72
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72
5	Hexacosane	366	C26H54	000630-01-3	52





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Acq On : 21 Apr 2021 12:56
Operator : JU/CG
Sample : M2076-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-17-0-2.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.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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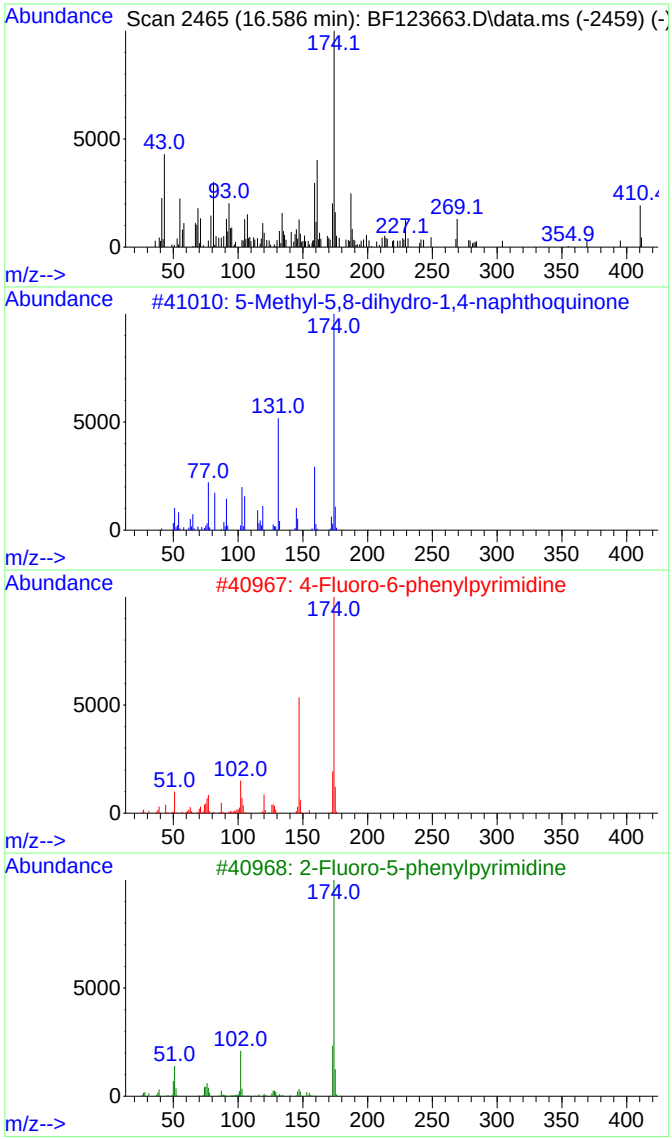
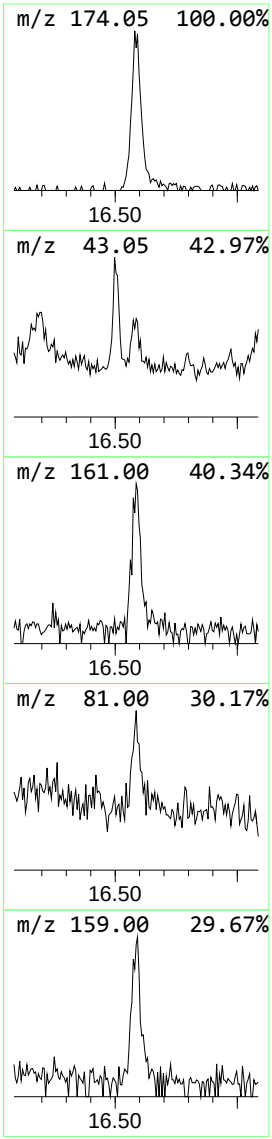
Peak Number 14 unknown16.58 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.586	5.07 ng	288329	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Methyl-5,8-dihydro-1,4-naphtho...	174	C11H10O2	086759-40-2	41
2	4-Fluoro-6-phenylpyrimidine	174	C10H7FN2	041270-94-4	35
3	2-Fluoro-5-phenylpyrimidine	174	C10H7FN2	062850-13-9	35
4	Pyrimido[1,6-a]indole, 1,2,3,4-t...	216	C13H16N2O	038349-09-6	32
5	6-Indolizinecarboxamide, 2-methyl-	174	C10H10N2O	022380-20-7	27





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Sample : M2076-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-17-0-2.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.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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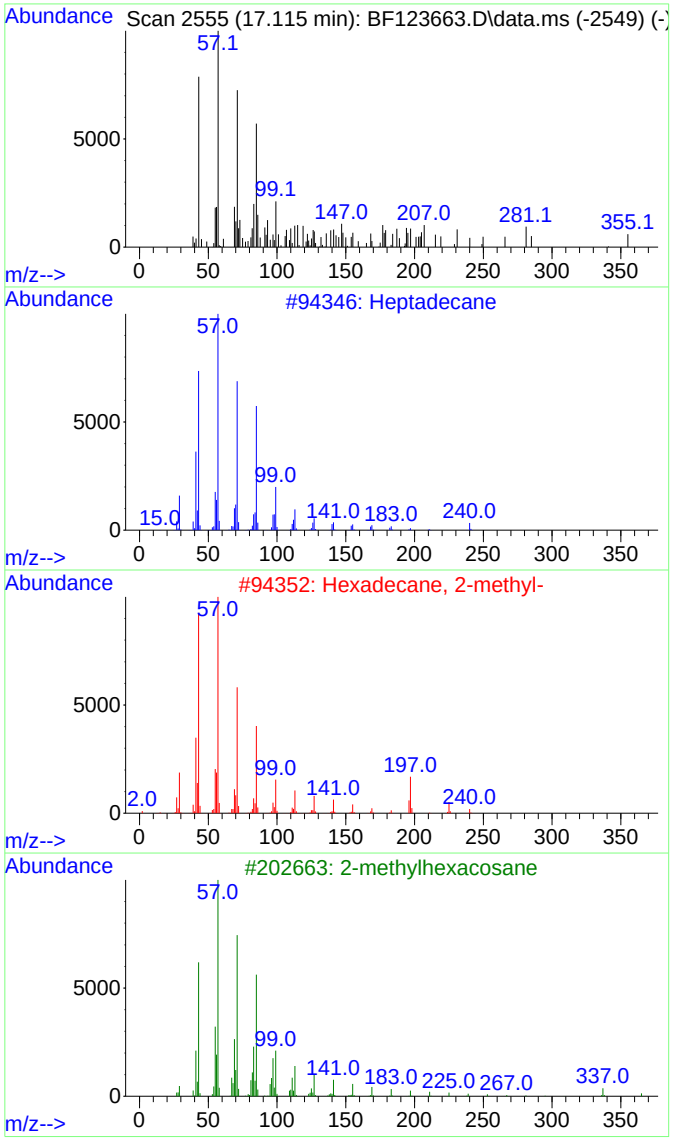
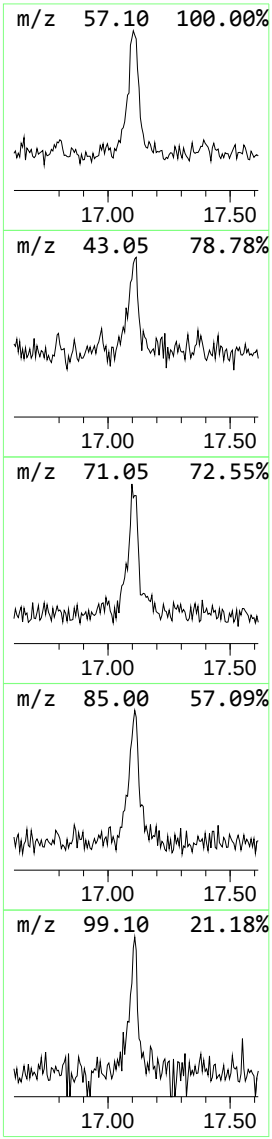
Peak Number 15 Hexadecane, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.115	2.73 ng	154994	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	70
2	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	58
3	2-methylhexacosane	380	C27H56	1000376-72-7	52
4	2-methyloctacosane	408	C29H60	1000376-72-8	52
5	10-Methylnonadecane	282	C20H42	056862-62-5	50





Tentatively Identified Compound (LSC) summary

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Data File : BF123663.D
Acq On : 21 Apr 2021 12:56
Operator : JU/CG
Sample : M2076-13
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-0-2.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.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
Dodecanoic acid	11.916	7.8	ng	708961	4	11.380	1813420	20.0
unknown12.30	12.304	2.3	ng	209898	4	11.380	1813420	20.0
Octadecanoic acid	12.704	12.4	ng	1124890	4	11.380	1813420	20.0
Heptadecane	13.351	3.0	ng	222364	5	14.027	1498090	20.0
Decanamide-	13.527	3.2	ng	239224	5	14.027	1498090	20.0
Diethylene glyc...	13.892	4.3	ng	319489	5	14.027	1498090	20.0
1-Docosene	13.933	9.7	ng	726816	5	14.027	1498090	20.0
Sulfurous acid,...	14.504	2.3	ng	172150	5	14.027	1498090	20.0
Sulfurous acid,...	14.768	2.6	ng	148216	6	15.509	1137530	20.0
Octacosane	14.815	3.9	ng	219257	6	15.509	1137530	20.0
2-methyloctacosane	15.156	5.9	ng	333227	6	15.509	1137530	20.0
Octadecane, 2-m...	15.992	5.9	ng	335648	6	15.509	1137530	20.0
Hexadecane, 6,1...	16.503	2.5	ng	142735	6	15.509	1137530	20.0
unknown16.58	16.586	5.1	ng	288329	6	15.509	1137530	20.0
Hexadecane, 2-m...	17.115	2.7	ng	154994	6	15.509	1137530	20.0