LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123654.D
Acq On : 20 Apr 2021 21:22
Operator : JU/CG
Sample : M2076-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-14.5-15.0

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: BF123654.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	500	506	512	rVB	71887	91459	1.47%	0.185%
2	5.469	571	575	579	rBV	6357205	6058652	97.51%	12.268%
3	6.016	663	668	672	rBV	65262	67058	1.08%	0.136%
4	6.487	743	748	753	rBV	6216228	6213505	100.00%	12.581%
5	6.845	806	809	817	rVB	1773803	1547002	24.90%	3.132%
6	7.028	837	840	843	rVB	129710	104557	1.68%	0.212%
7	7.410	900	905	908	rBV	4526520	4050802	65.19%	8.202%
8	7.492	915	919	924	rVB4	51681	71601	1.15%	0.145%
9	8.134	1024	1028	1031	rBV	2530937	1989832	32.02%	4.029%
10	9.210	1207	1211	1214	rBV	6879387	6160992	99.15%	12.475%
11	9.292	1222	1225	1229	rBV2	73553	72695	1.17%	0.147%
12	9.604	1275	1278	1282	rBV	308686	261275	4.20%	0.529%
13	9.892	1323	1327	1330	rBV	2558351	2047316	32.95%	4.145%
14	10.092	1357	1361	1364	rBV3	67919	65650	1.06%	0.133%
15	10.680	1457	1461	1464	rBV	4927421	4179802	67.27%	8.463%
16	11.251	1551	1558	1560	rBV5	42291	79737	1.28%	0.161%
17	11.380	1576	1580	1582	rBV	2534689	2098075	33.77%	4.248%
18	11.404	1582	1584	1587	rVV	372399	285580	4.60%	0.578%
19	11.451	1587	1592	1596	rVB2	121917	143661	2.31%	0.291%
20	11.910	1667	1670	1675	rBV2	393952	374762	6.03%	0.759%
21	11.992	1681	1684	1687	rBV	77029	88239	1.42%	0.179%
22	12.363	1744	1747	1749	rBV2	67040	68283	1.10%	0.138%
23	12.598	1784	1787	1790	rBV	650508	510289	8.21%	1.033%
24	12.821	1819	1825	1828	rBV2	506397	569783	9.17%	1.154%
25	12.851	1828	1830	1840	rVB3	142518	263032	4.23%	0.533%
26	12.974	1846	1851	1854	rVB	5432780	5160587	83.05%	10.449%
27	13.151	1879	1881	1885	rVB2	97515	101602	1.64%	0.206%
28	13.204	1888	1890	1892	rVV	91655	100262	1.61%	0.203%
29	13.257	1896	1899	1902	rVB3	74956	77470	1.25%	0.157%
30	13.663	1965	1968	1973	rVB	77431	83710	1.35%	0.169%
31	13.880	2002	2005	2021	rVB2	464494	947243	15.24%	1.918%
32	14.021	2025	2029	2032	rVV2	1554204	1710139	27.52%	3.463%
33	14.051	2032	2034	2036	rVB	278440	211367	3.40%	0.428%
34	14.198	2056	2059	2064	rBV2	70515	97806	1.57%	0.198%
35	14.504	2108	2111	2113	rBV2	97271	78201	1.26%	0.158%
36	14.815	2161	2164	2166	rBV2	76129	79546	1.28%	0.161%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
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Acq On : 20 Apr 2021 21:22
Operator : JU/CG
Sample : M2076-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-14.5-15.0

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

37	15.068	2204	2207	2210	rBV	220990	317639	5.11%	0.643%
38	15.157	2219	2222	2224	rBV2	104567	110535	1.78%	0.224%
39	15.374	2256	2259	2266	rVB	160339	218159	3.51%	0.442%
40	15.439	2266	2270	2276	rBV	215514	272386	4.38%	0.552%
41	15.504	2276	2281	2285	rVV	1126773	1450628	23.35%	2.937%
42	15.539	2285	2287	2292	rVB4	159467	194290	3.13%	0.393%
43	15.745	2320	2322	2327	rVB5	68141	71550	1.15%	0.145%
44	15.986	2359	2363	2368	rBV3	138298	207272	3.34%	0.420%
45	16.227	2400	2404	2412	rVB3	91638	190819	3.07%	0.386%
46	16.498	2448	2450	2454	rBV3	54294	68475	1.10%	0.139%
47	16.798	2497	2501	2506	rVB6	94936	174218	2.80%	0.353%

Sum of corrected areas: 49387543

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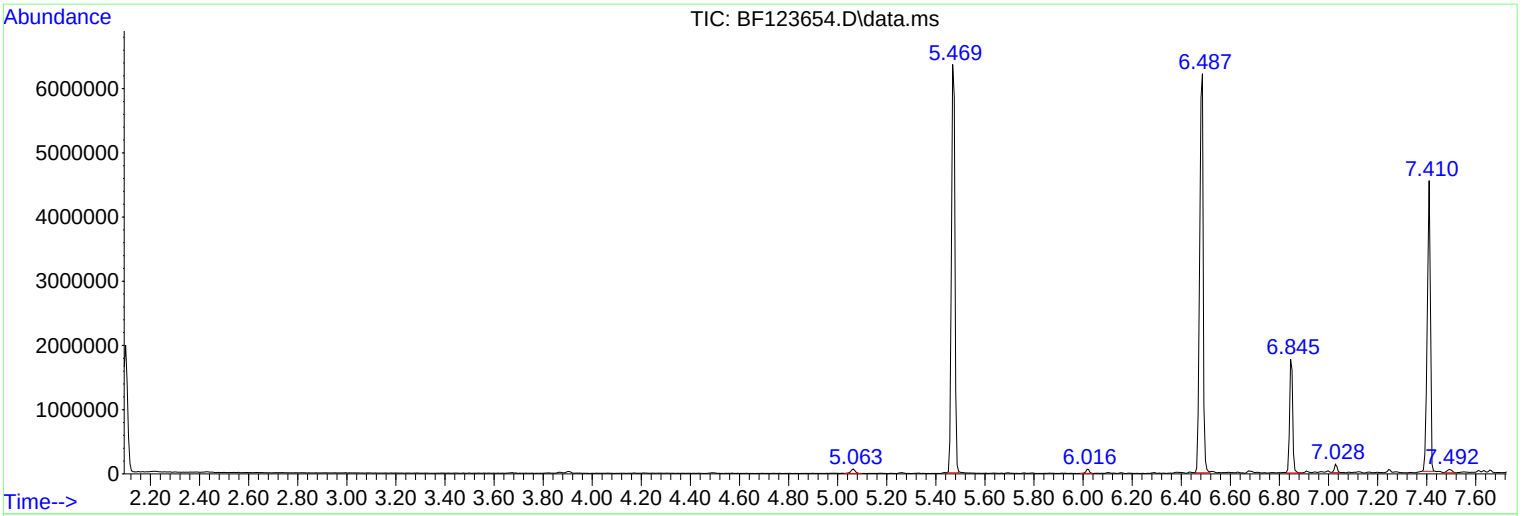
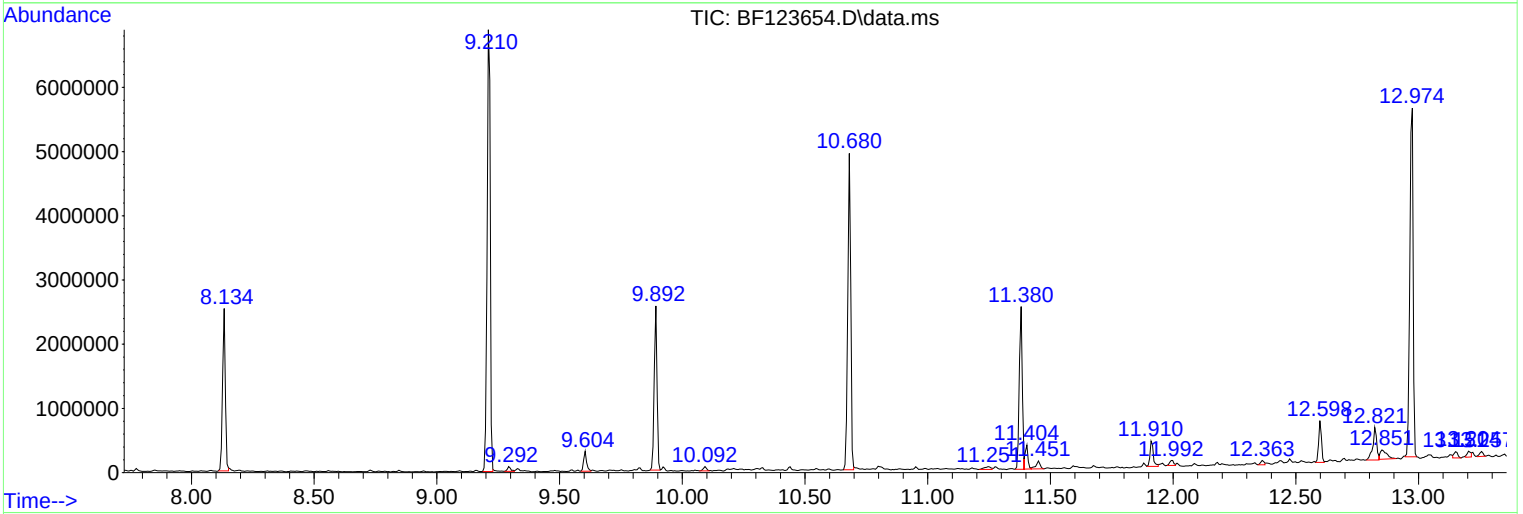
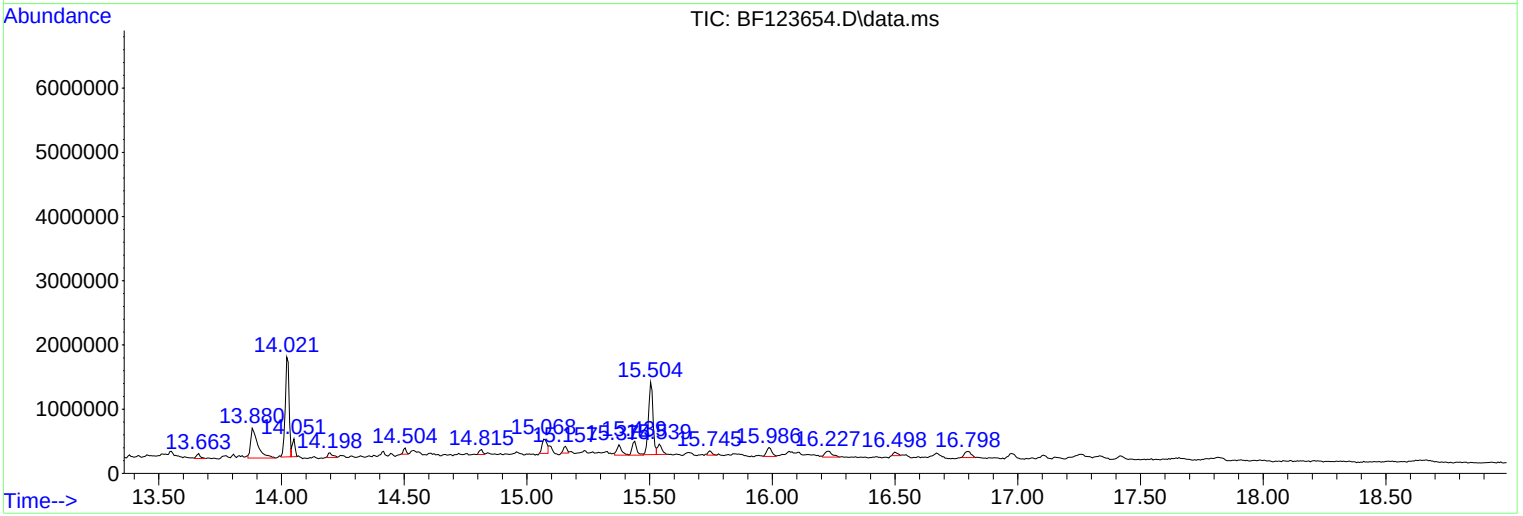
Instrument :
BNA_F
ClientSampleId :
SB-17-14.5-15.0

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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Data File : BF123654.D
Acq On : 20 Apr 2021 21:22
Operator : JU/CG
Sample : M2076-15
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Instrument :
BNA_F
ClientSampleId :
SB-17-14.5-15.0

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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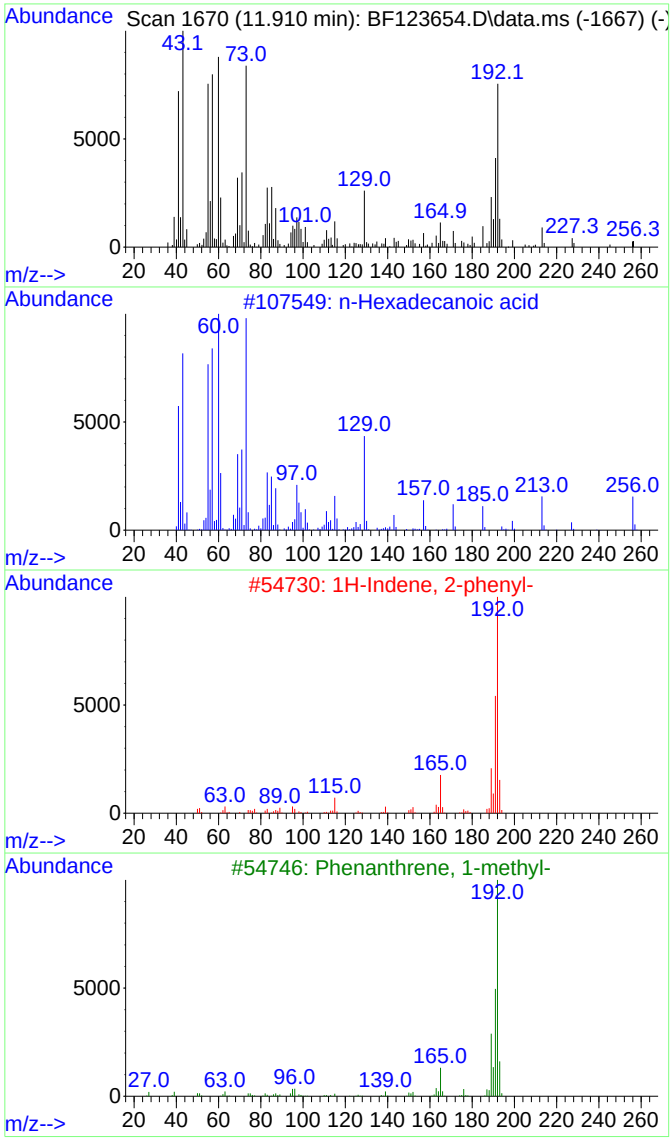
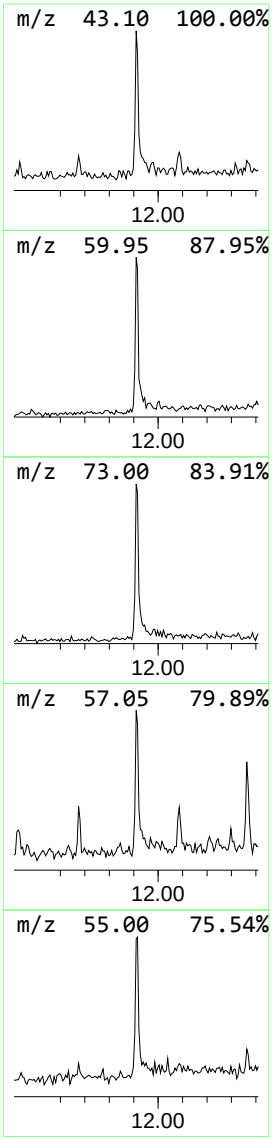
Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.910	3.57 ng	374762	Phenanthrene-d10	11.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	74
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	72
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	70
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	55





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Data File : BF123654.D
Acq On : 20 Apr 2021 21:22
Operator : JU/CG
Sample : M2076-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-17-14.5-15.0

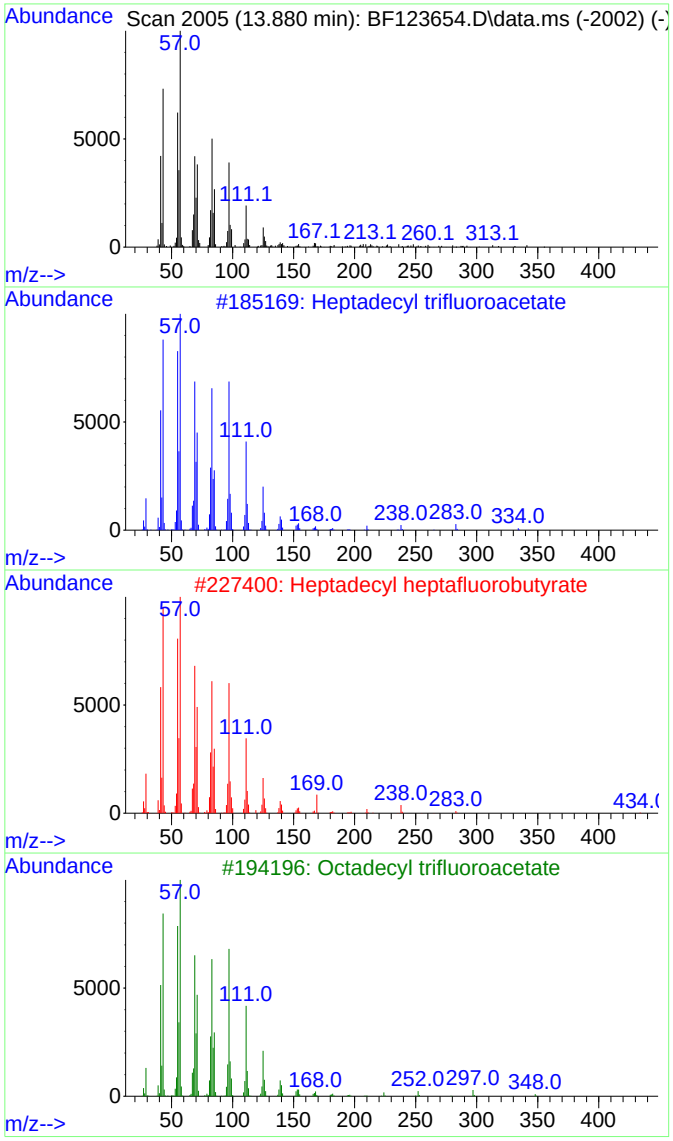
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

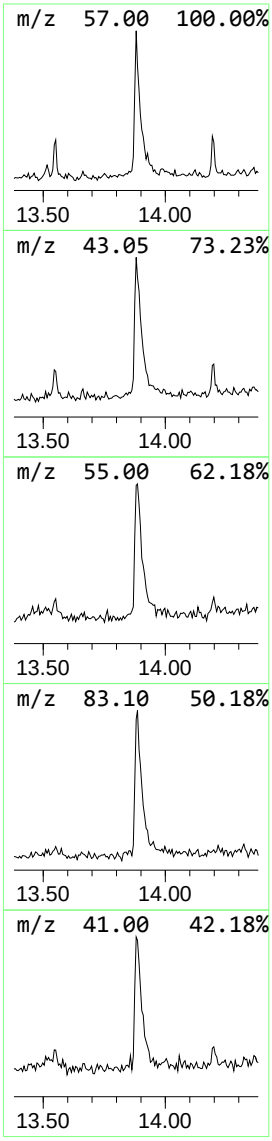
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Heptadecyl trifluoroacetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	11.08 ng	947243	Chrysene-d12	14.027

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123654.D
Acq On : 20 Apr 2021 21:22
Operator : JU/CG
Sample : M2076-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-17-14.5-15.0

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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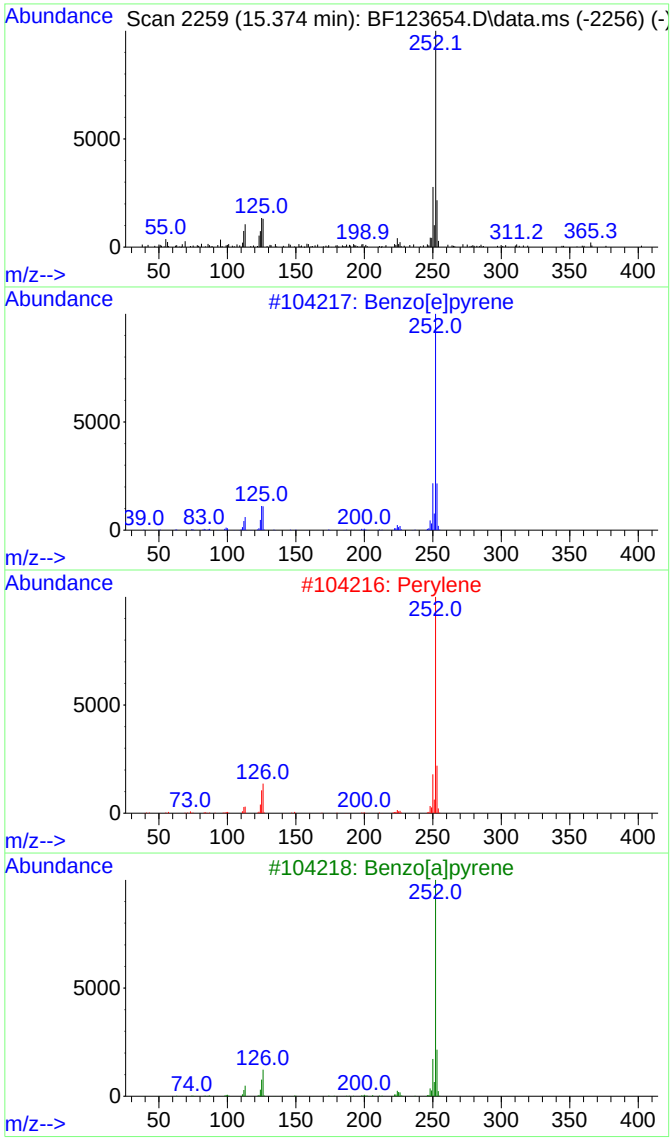
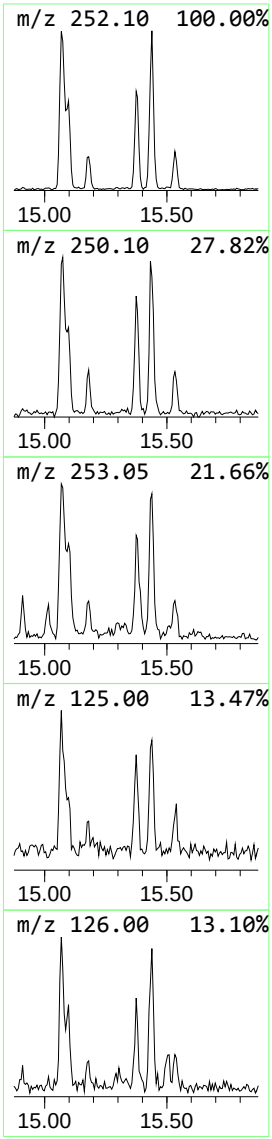
Peak Number 3 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.374	3.01 ng	218159	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Perylene	252	C20H12	000198-55-0	94
3	Benzo[a]pyrene	252	C20H12	000050-32-8	94
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123654.D
Acq On : 20 Apr 2021 21:22
Operator : JU/CG
Sample : M2076-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-17-14.5-15.0

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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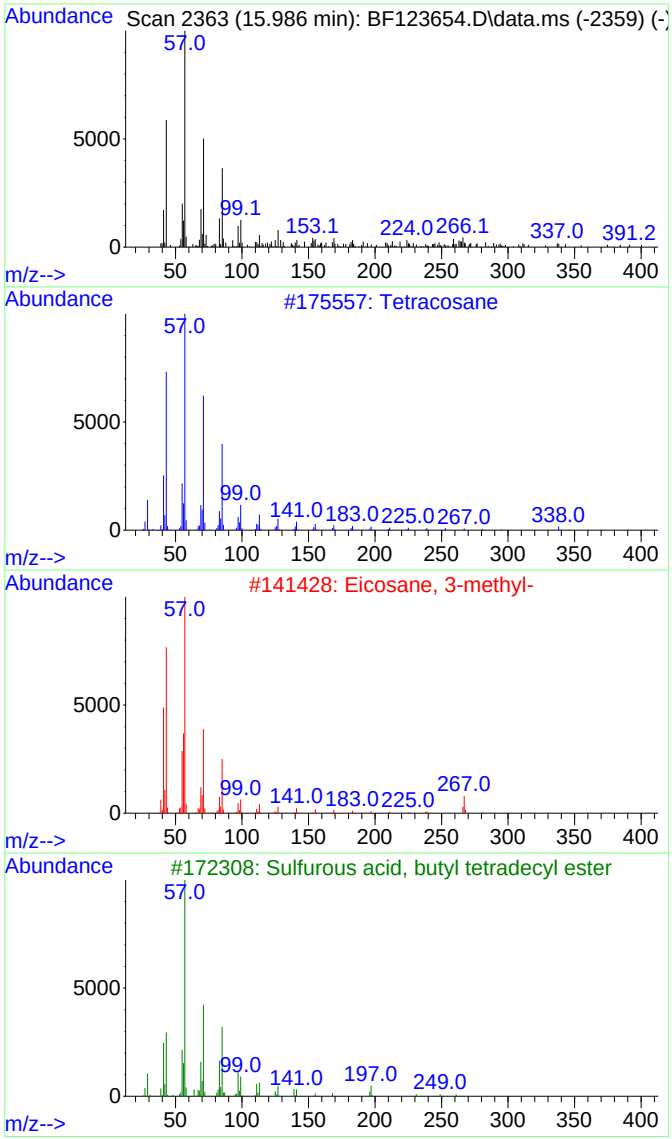
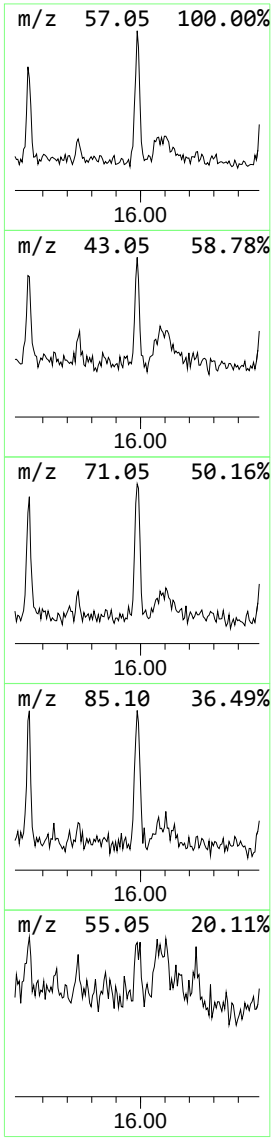
Peak Number 4 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.986	2.86 ng	207272	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Eicosane, 3-methyl-	296	C21H44	006418-46-8	86
3	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	80
4	Tetradecane, 3-methyl-	212	C15H32	018435-22-8	76
5	Hexadecane	226	C16H34	000544-76-3	76





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Sample : M2076-15
Misc :
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Instrument :
BNA_F
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SB-17-14.5-15.0

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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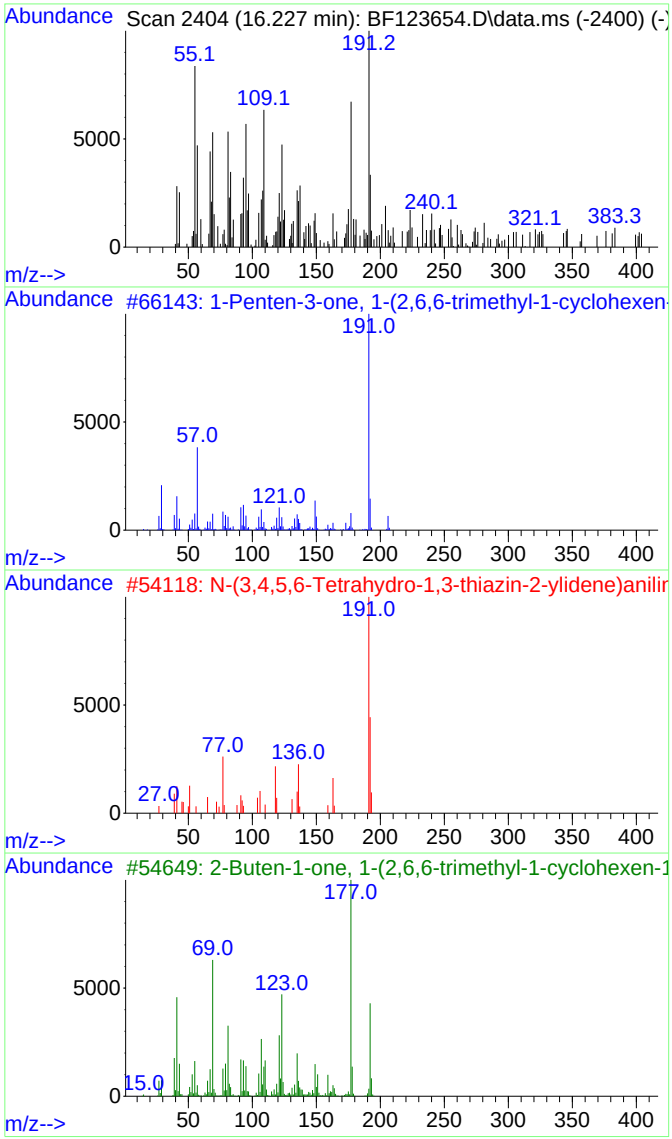
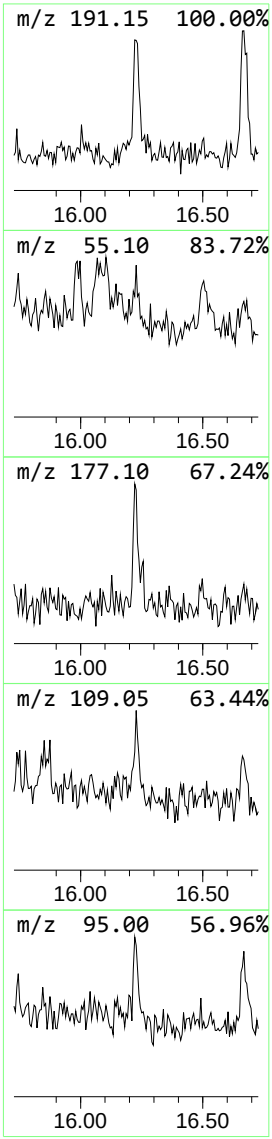
Peak Number 5 unknown16.227 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.227	2.63 ng	190819	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	30
2	N-(3,4,5,6-Tetrahydro-1,3-thiazi...	192	C10H12N2S	003420-40-4	30
3	2-Buten-1-one, 1-(2,6,6-trimethy...	192	C13H20O	035044-68-9	30
4	2-Phenylamino-5,6(4H)dihydro-1,3...	192	C10H12N2S	1000147-35-4	25
5	5-Hexen-1-one, 1-(1H-imidazol-4-...	192	C11H16N2O	069393-41-5	25





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Misc :
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Instrument :
BNA_F
ClientSampleId :
SB-17-14.5-15.0

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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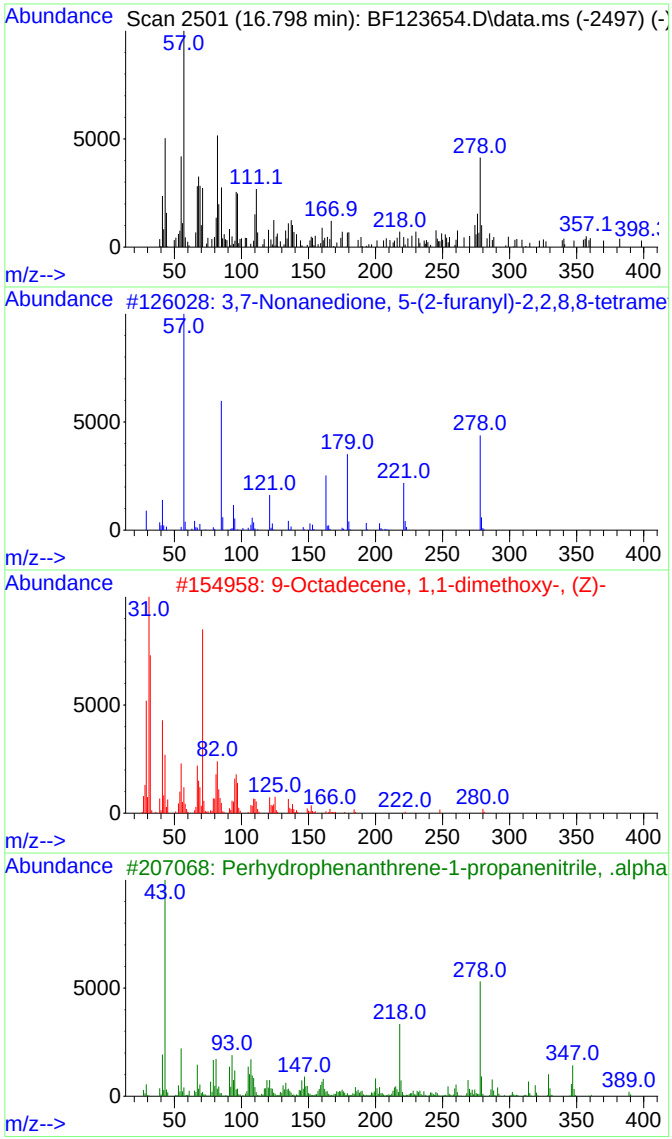
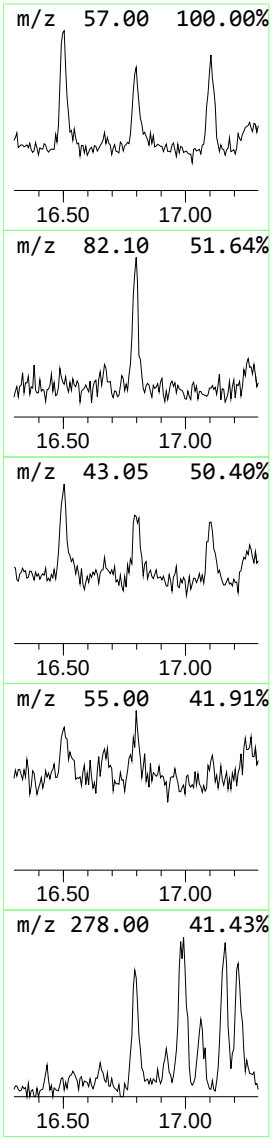
Peak Number 6 unknown16.798 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.798	2.40 ng	174218	Perylene-d12	15.504

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7-Nonanedione, 5-(2-furanyl)-2...	278	C17H26O3	1000319-41-4	22
2	9-Octadecene, 1,1-dimethoxy-, (Z)-	312	C20H40O2	015677-71-1	10
3	Perhydrophenanthrene-1-propaneni...	389	C22H31NO5	1000197-35-9	9
4	Acetamide, N-(3-ethyl-1-phenylin...	278	C18H18N2O	138349-53-8	9
5	6-Undecen-3-one, 5-butyl-2,2-dim...	252	C17H32O	055976-05-1	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042021\
Data File : BF123654.D
Acq On : 20 Apr 2021 21:22
Operator : JU/CG
Sample : M2076-15
Misc :
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Instrument : BNA_F
ClientSampleId : SB-17-14.5-15.0

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
n-Hexadecanoic ...	11.910	3.6	ng	374762	4	11.380	2098080	20.0
Heptadecyl trif...	13.880	11.1	ng	947243	5	14.027	1710140	20.0
Benzo[e]pyrene	15.374	3.0	ng	218159	6	15.504	1450630	20.0
Tetracosane	15.986	2.9	ng	207272	6	15.504	1450630	20.0
unknown16.227	16.227	2.6	ng	190819	6	15.504	1450630	20.0
unknown16.798	16.798	2.4	ng	174218	6	15.504	1450630	20.0