LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119453.D
Acq On : 19 Mar 2020 22:22
Operator : CG/JU
Sample : L1913-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MK-031220-0-2-COMP-B1

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-BF031820.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	15	rVB	235839	332206	4.79%	0.546%
2	3.310	204	208	221	rBV	27864	70800	1.02%	0.116%
3	5.063	500	506	513	rVB	77251	105607	1.52%	0.174%
4	5.457	568	573	576	rBV	6228902	6336881	91.42%	10.417%
5	6.469	739	745	748	rBV	5994380	6278180	90.57%	10.320%
6	6.669	776	779	782	rBV	214996	154766	2.23%	0.254%
7	6.845	806	809	813	rBV	2233537	1941604	28.01%	3.192%
8	7.004	832	836	839	rBV	5947491	5020726	72.43%	8.253%
9	7.410	900	905	908	rBV	4483204	4159093	60.00%	6.837%
10	8.134	1023	1028	1031	rBV	3118719	2583250	37.27%	4.246%
11	9.210	1206	1211	1215	rBV	7236291	6931884	100.00%	11.395%
12	9.604	1274	1278	1281	rBV	1182643	879496	12.69%	1.446%
13	9.892	1320	1327	1330	rBV	3420638	2847715	41.08%	4.681%
14	10.680	1455	1461	1464	rBV	4480317	4134140	59.64%	6.796%
15	11.380	1575	1580	1582	rBV	3122839	2740270	39.53%	4.504%
16	11.398	1582	1583	1587	rVV	413436	329398	4.75%	0.541%
17	11.451	1587	1592	1595	rVB	120446	124686	1.80%	0.205%
18	11.910	1667	1670	1675	rBV	521065	493163	7.11%	0.811%
19	11.992	1680	1684	1686	rBV2	104612	99124	1.43%	0.163%
20	12.433	1755	1759	1762	rBV2	68197	79286	1.14%	0.130%
21	12.592	1782	1786	1789	rBV	819960	663347	9.57%	1.090%
22	12.692	1800	1803	1810	rBV3	149388	194795	2.81%	0.320%
23	12.821	1819	1825	1828	rBV	683390	678222	9.78%	1.115%
24	12.968	1846	1850	1853	rBV	6116962	5311322	76.62%	8.731%
25	13.039	1857	1862	1865	rBV2	49942	73763	1.06%	0.121%
26	13.151	1878	1881	1883	rVB	98550	85602	1.23%	0.141%
27	13.216	1888	1892	1895	rVB2	96505	85808	1.24%	0.141%
28	13.251	1895	1898	1902	rBV	64294	76873	1.11%	0.126%
29	13.833	1993	1997	1999	rBV2	95631	117579	1.70%	0.193%
30	13.868	1999	2003	2010	rVB2	609364	668216	9.64%	1.098%
31	14.021	2024	2029	2031	rBV2	2054099	2095552	30.23%	3.445%
32	14.045	2031	2033	2039	rVB	326586	287972	4.15%	0.473%
33	14.198	2056	2059	2063	rVB2	109873	112358	1.62%	0.185%
34	14.498	2107	2110	2114	rBV3	179800	201226	2.90%	0.331%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119453.D
Acq On : 19 Mar 2020 22:22
Operator : CG/JU
Sample : L1913-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MK-031220-0-2-COMP-B1

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-BF031820.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.651	2132	2136	2138	rBV2	146480	168564	2.43%	0.277%
36	14.810	2160	2163	2169	rVB	162412	188449	2.72%	0.310%
37	14.886	2173	2176	2182	rVB2	118957	152330	2.20%	0.250%
38	15.057	2201	2205	2208	rBV	295115	416307	6.01%	0.684%
39	15.157	2218	2222	2229	rVB2	186044	282310	4.07%	0.464%
40	15.362	2253	2257	2263	rVB	179075	235231	3.39%	0.387%
41	15.421	2263	2267	2273	rBV	263423	327714	4.73%	0.539%
42	15.492	2274	2279	2283	rVV	1501493	1852879	26.73%	3.046%
43	15.539	2285	2287	2291	rVB2	155471	176723	2.55%	0.290%
44	15.980	2358	2362	2367	rBV2	111595	176592	2.55%	0.290%
45	16.033	2367	2371	2379	rVB8	69823	146051	2.11%	0.240%
46	16.945	2521	2526	2534	rVB2	139550	274413	3.96%	0.451%
47	17.386	2597	2601	2607	rVB	86556	141616	2.04%	0.233%

Sum of corrected areas: 60834089

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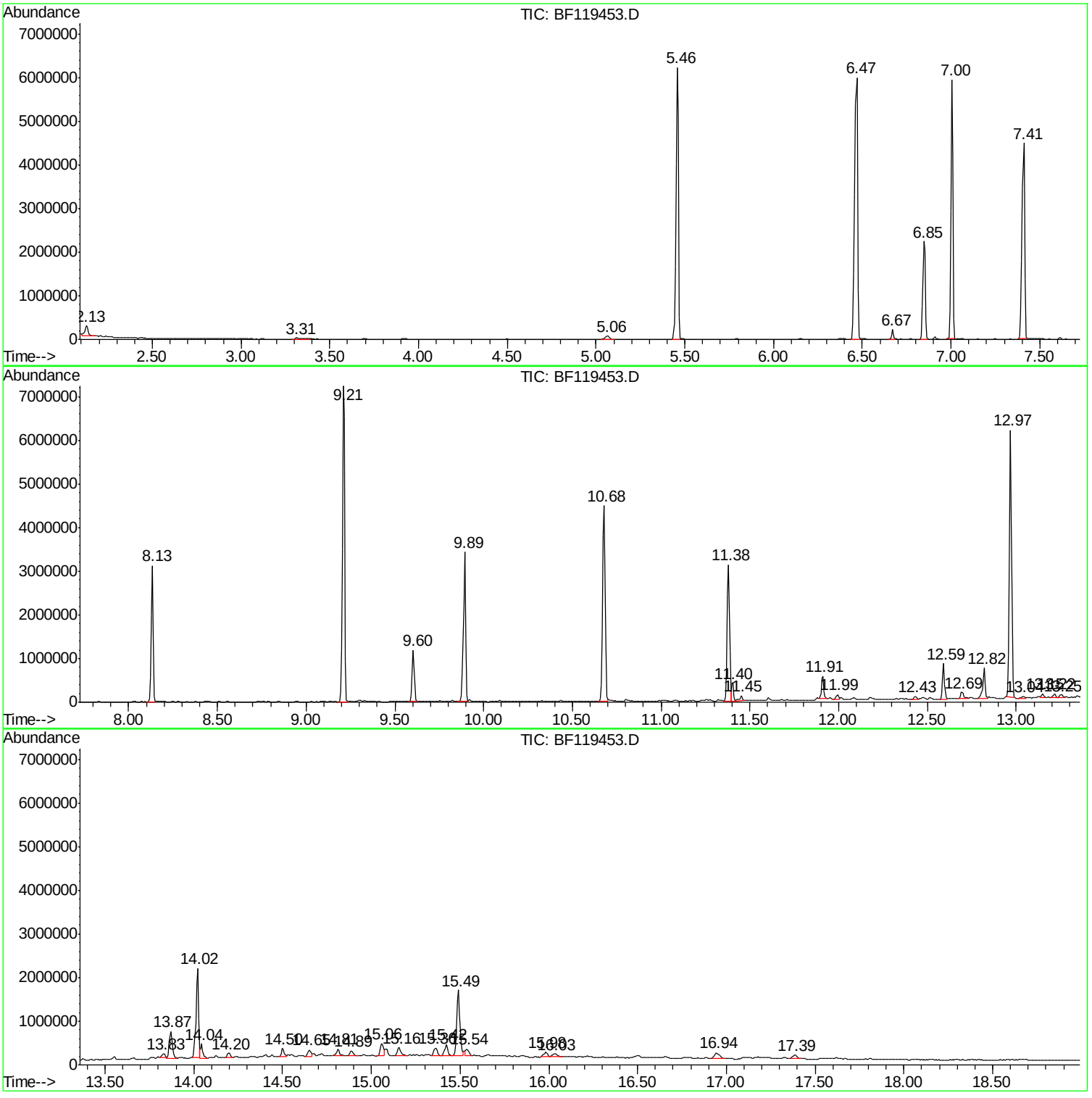
Instrument :
BNA_F
ClientSampleId :
MK-031220-0-2-COMP-B1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119453.D
Acq On : 19 Mar 2020 22:22
Operator : CG/JU
Sample : L1913-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MK-031220-0-2-COMP-B1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

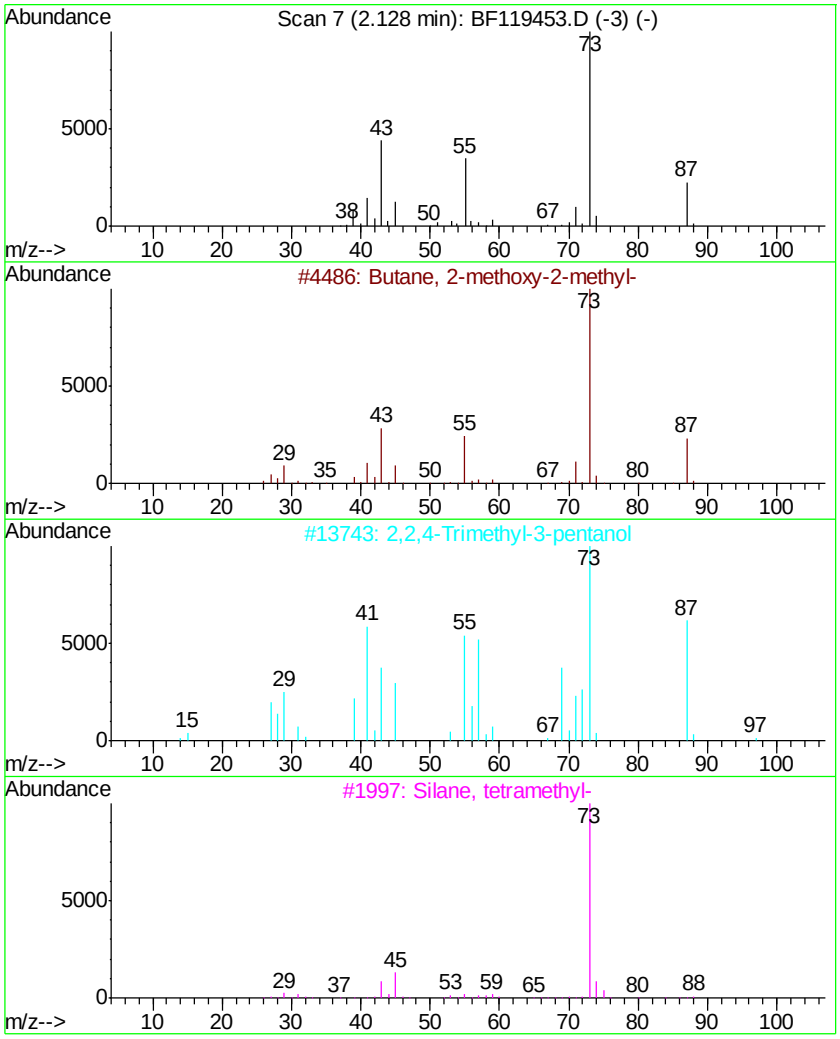
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

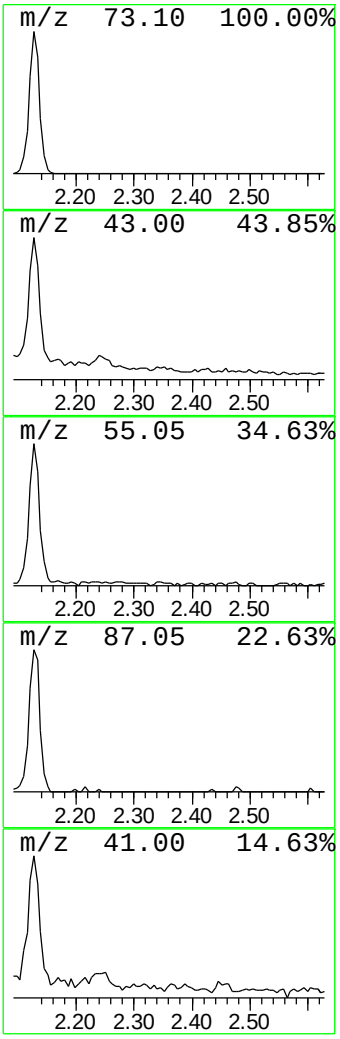
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	3.42 ng	332206	1,4-Dichlorobenzene-d4	6.85

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	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119453.D
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Operator : CG/JU
Sample : L1913-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MK-031220-0-2-COMP-B1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

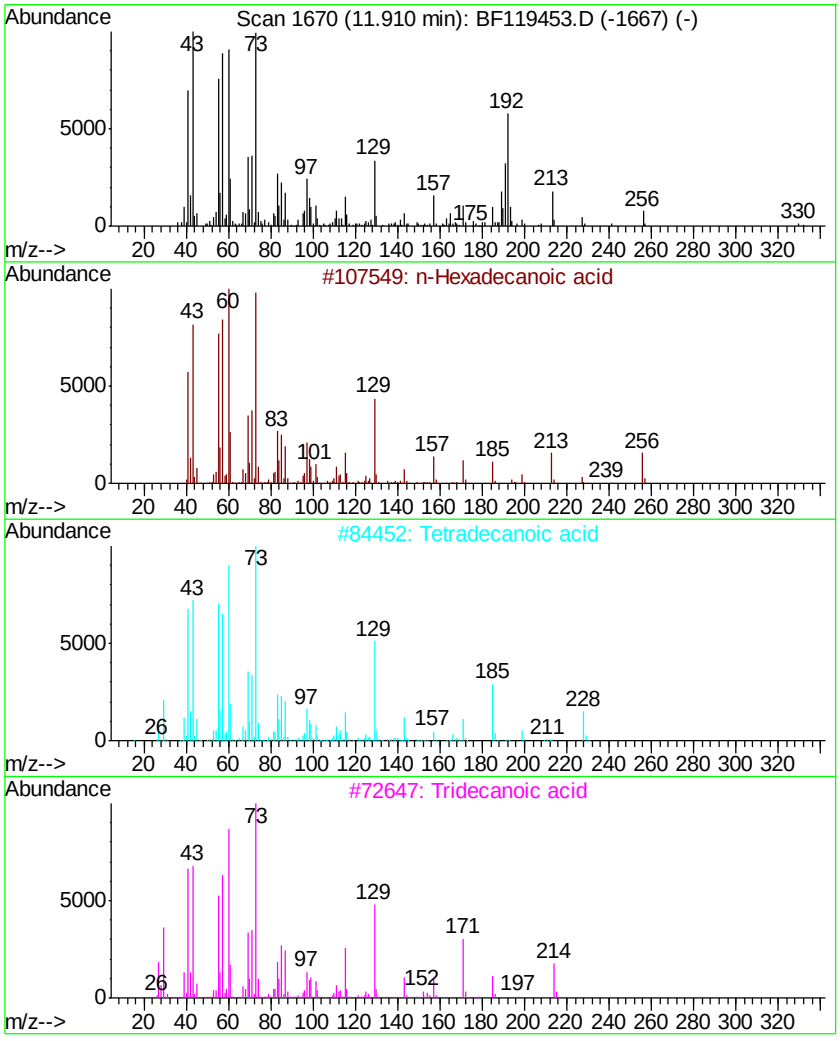
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

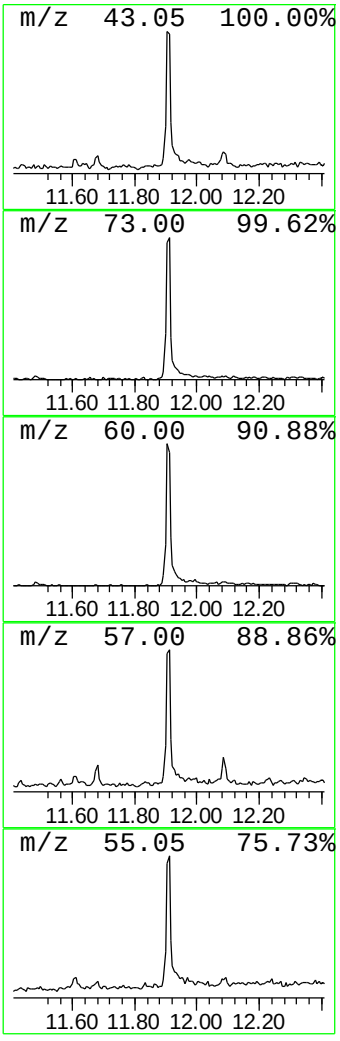
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	3.60 ng	493163	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	96
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	80
5	Octadecanoic acid	284	C18H36O2	000057-11-4	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119453.D
Acq On : 19 Mar 2020 22:22
Operator : CG/JU
Sample : L1913-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MK-031220-0-2-COMP-B1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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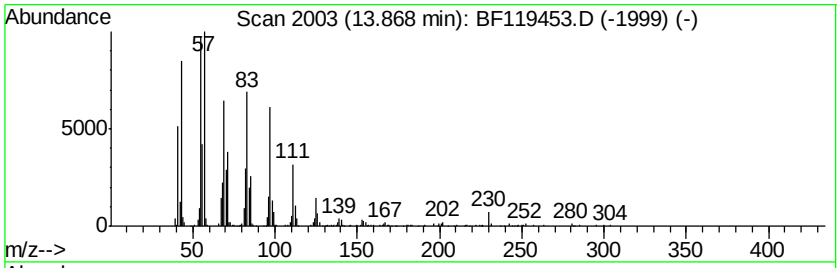
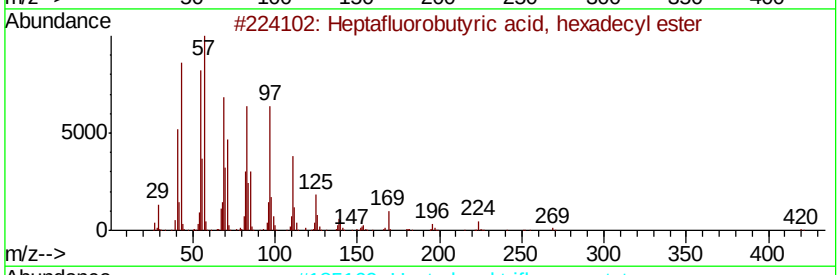
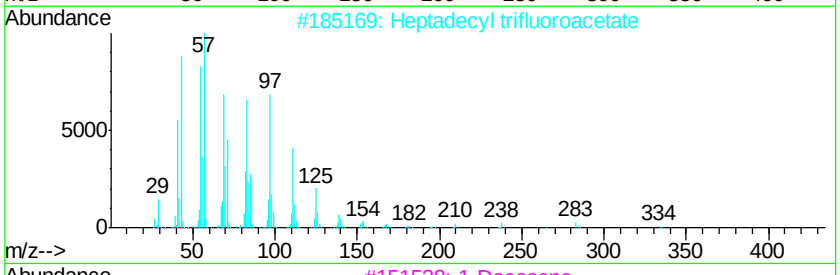
Peak Number 4 Heptafluorobutyric acid, he... Concentration Rank 2

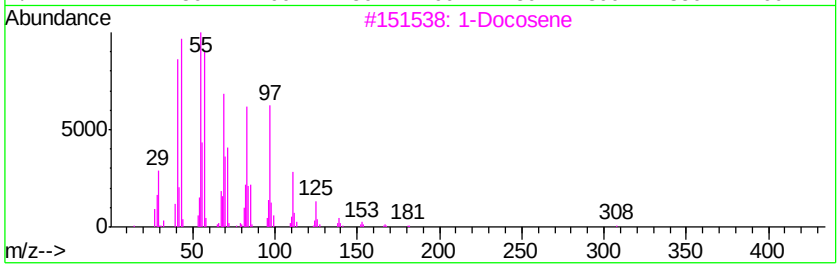
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	6.38 ng	668216	Chrysene-d12	14.02

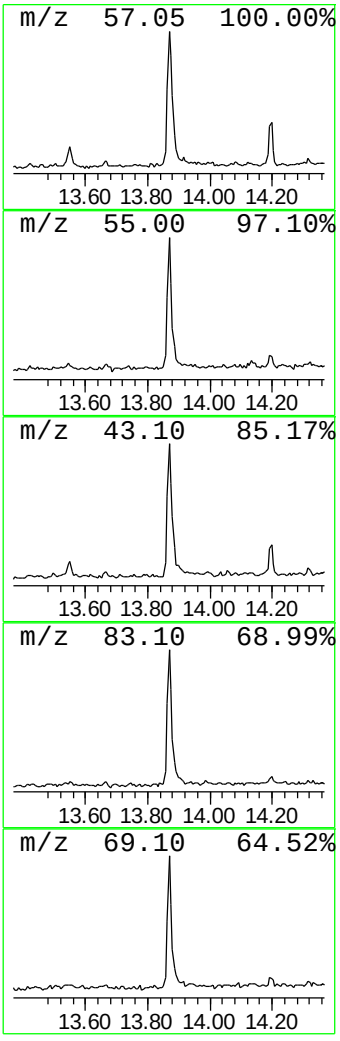
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3	1-Docosene	308	C22H44	001599-67-3	94
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91











Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119453.D
Acq On : 19 Mar 2020 22:22
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Sample : L1913-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MK-031220-0-2-COMP-B1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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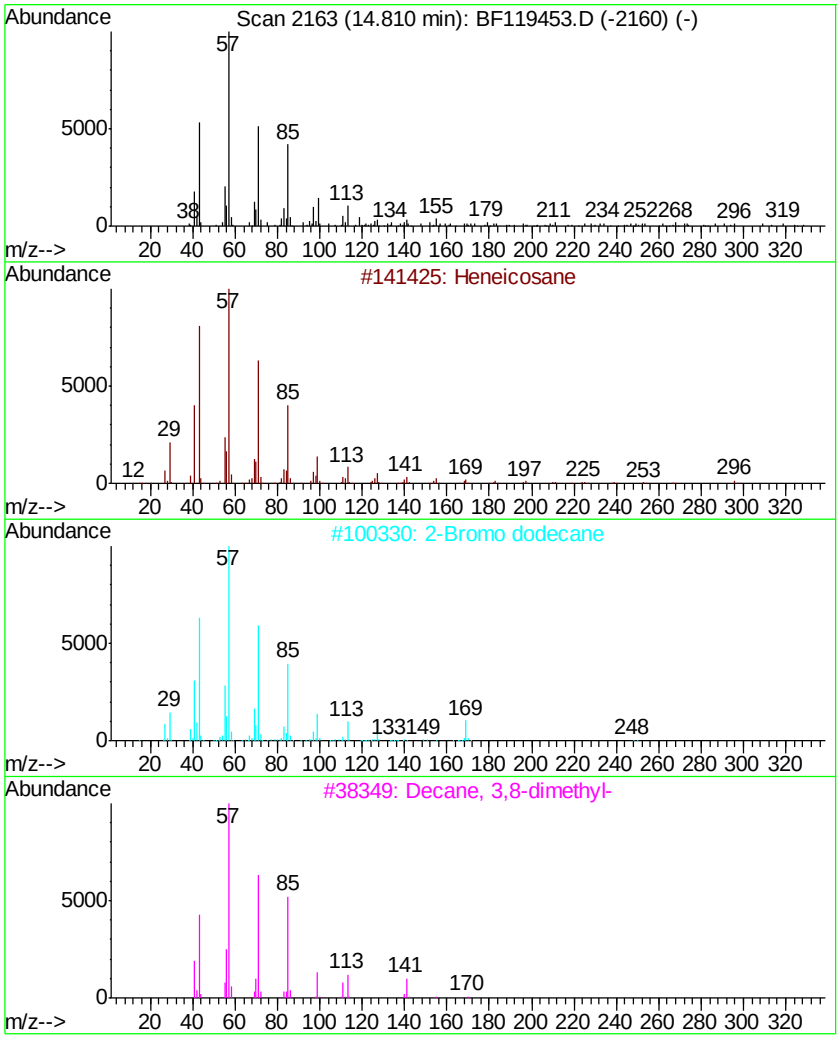
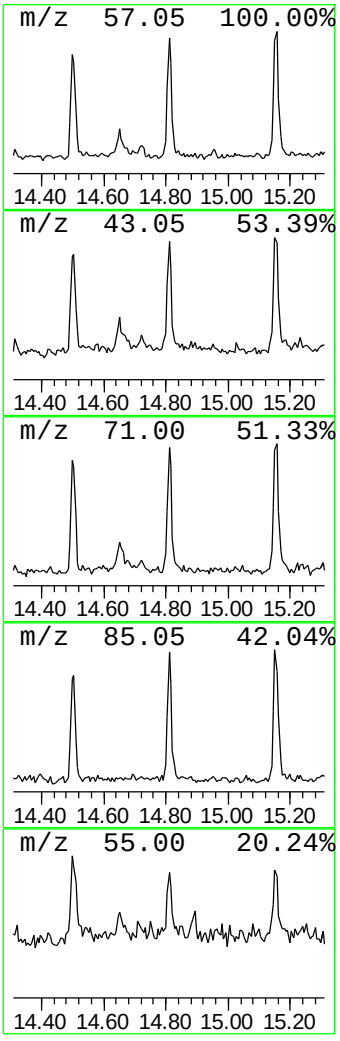
Peak Number 5 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	2.03 ng	188449	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	96
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	91
3	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	91
4	Octacosane	394	C28H58	000630-02-4	90
5	Tricosane	324	C23H48	000638-67-5	87





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Data File : BF119453.D
Acq On : 19 Mar 2020 22:22
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Sample : L1913-02
Misc :
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Instrument : BNA_F
ClientSampleId : MK-031220-0-2-COMP-B1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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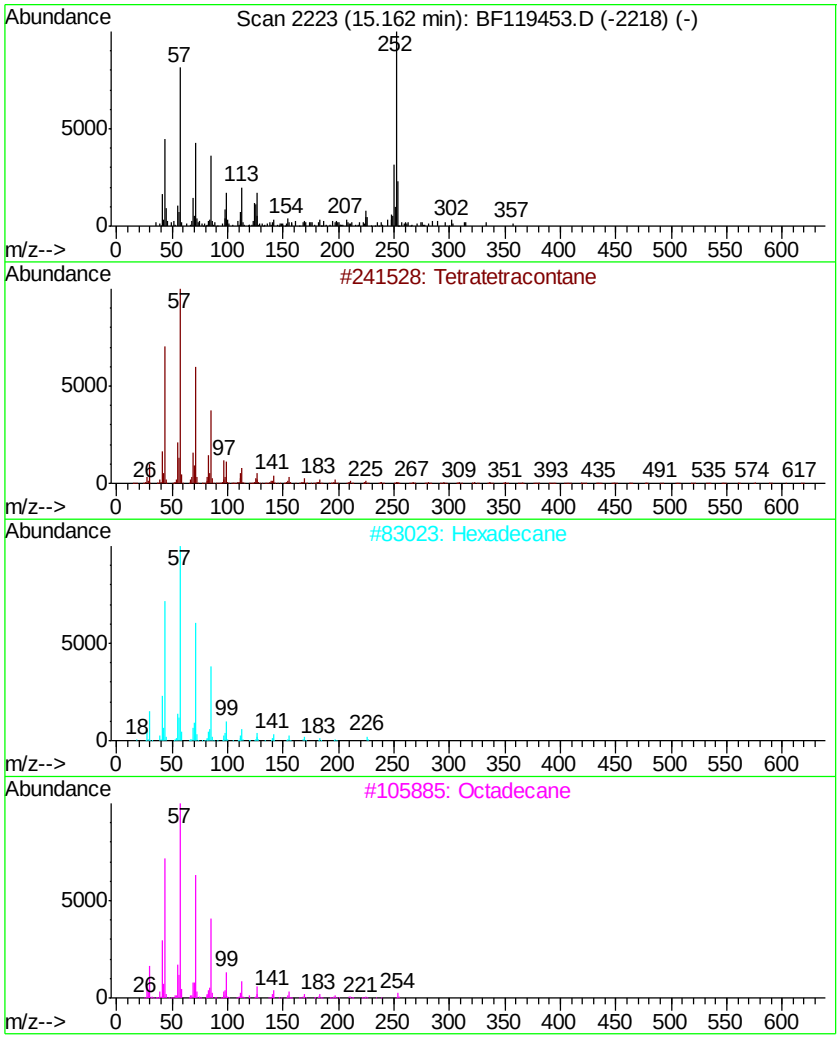
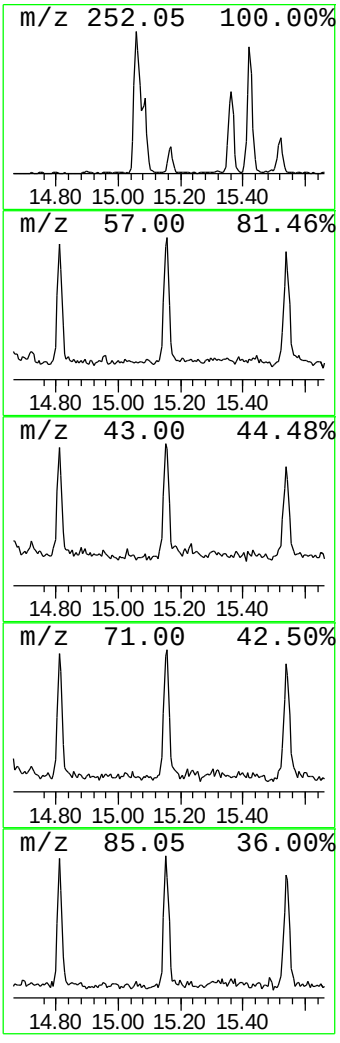
Peak Number 6 Tetratetracontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	3.05 ng	282310	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	68
2	Hexadecane	226	C16H34	000544-76-3	64
3	Octadecane	254	C18H38	000593-45-3	64
4	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	64
5	Docosane	310	C22H46	000629-97-0	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031920\
Data File : BF119453.D
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Operator : CG/JU
Sample : L1913-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MK-031220-0-2-COMP-B1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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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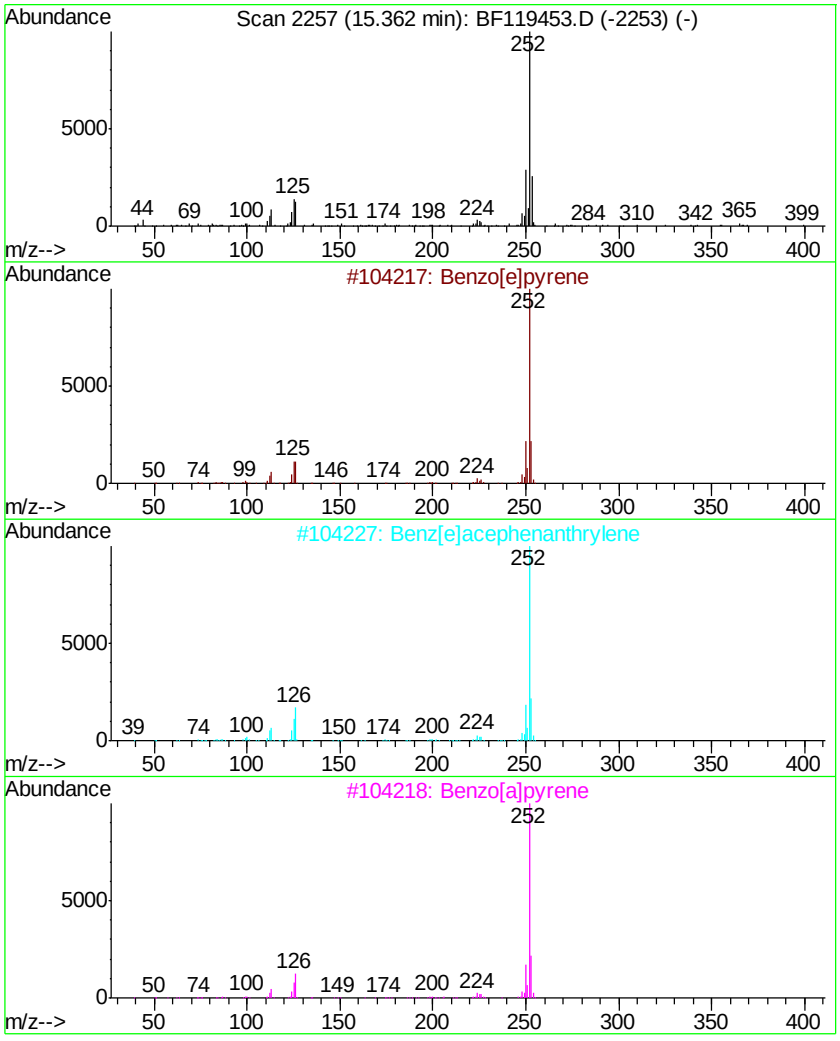
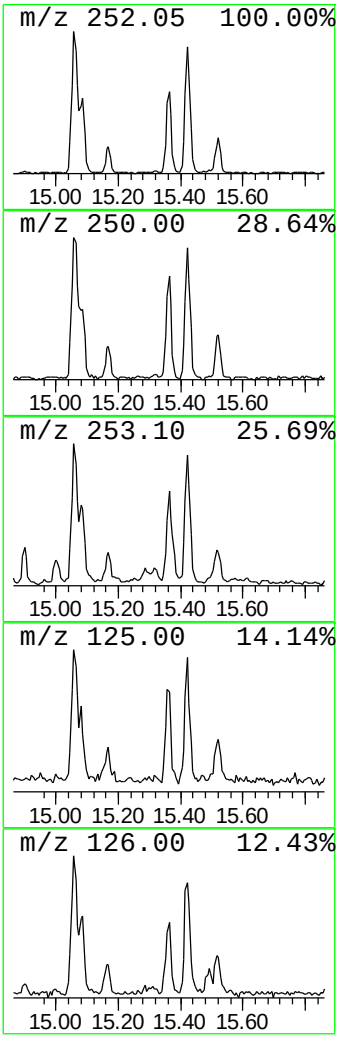
Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	2.54 ng	235231	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
3	Benzo[a]pyrene	252	C20H12	000050-32-8	94
4	Perylene	252	C20H12	000198-55-0	94
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031920\
Data File : BF119453.D
Acq On : 19 Mar 2020 22:22
Operator : CG/JU
Sample : L1913-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MK-031220-0-2-COMP-B1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF031820.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-methoxy...	2.13	3.4	ng	332206	1	6.85	1941600	20.0
n-Hexadecanoic acid	11.91	3.6	ng	493163	4	11.38	2740270	20.0
Heptafluorobutyri...	13.87	6.4	ng	668216	5	14.02	2095550	20.0
Heneicosane	14.81	2.0	ng	188449	6	15.49	1852880	20.0
Tetratetracontane	15.16	3.0	ng	282310	6	15.49	1852880	20.0
Benzo[e]pyrene	15.36	2.5	ng	235231	6	15.49	1852880	20.0