LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119659.D
Acq On : 31 Mar 2020 18:34
Operator : MA/SJ
Sample : L2055-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6-(1-3)

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	2.204	16	20	27	rVB	136901	180544	2.66%	0.284%
2	5.045	497	503	510	rVB	191409	232075	3.41%	0.365%
3	5.445	566	571	574	rBV	6712216	6675117	98.17%	10.501%
4	6.457	737	743	746	rBV	5949162	6663338	97.99%	10.482%
5	6.828	803	806	810	rBV	2294679	1854079	27.27%	2.917%
6	6.986	829	833	836	rBV	6290295	5308993	78.08%	8.352%
7	7.392	894	902	905	rBV	4655284	4362372	64.15%	6.863%
8	8.116	1021	1025	1027	rBV	2856667	2308592	33.95%	3.632%
9	8.133	1027	1028	1034	rVB	241985	175554	2.58%	0.276%
10	8.828	1143	1146	1149	rVB	127071	94971	1.40%	0.149%
11	9.198	1203	1209	1212	rBV	8051118	6799776	100.00%	10.697%
12	9.586	1272	1275	1280	rBV	1021191	883127	12.99%	1.389%
13	9.733	1297	1300	1304	rBV	357445	309011	4.54%	0.486%
14	9.875	1319	1324	1328	rBV	2709115	2294804	33.75%	3.610%
15	10.080	1355	1359	1361	rBV2	83658	81273	1.20%	0.128%
16	10.669	1454	1459	1462	rBV	3832022	3464001	50.94%	5.449%
17	10.769	1473	1476	1478	rBV	178134	152978	2.25%	0.241%
18	10.786	1478	1479	1487	rVB3	116542	151336	2.23%	0.238%
19	11.027	1518	1520	1524	rBV	100872	97129	1.43%	0.153%
20	11.369	1574	1578	1580	rBV	2100132	1932795	28.42%	3.041%
21	11.392	1580	1582	1585	rVV	483632	381252	5.61%	0.600%
22	11.439	1585	1590	1593	rVB	264152	238984	3.51%	0.376%
23	11.469	1593	1595	1600	rBV3	100010	117770	1.73%	0.185%
24	11.821	1652	1655	1660	rBV	163001	209373	3.08%	0.329%
25	11.868	1660	1663	1665	rBV	121416	90613	1.33%	0.143%
26	11.898	1665	1668	1674	rBV	1574942	1511079	22.22%	2.377%
27	11.980	1679	1682	1685	rBV	182147	201102	2.96%	0.316%
28	12.421	1754	1757	1760	rBV	133536	124348	1.83%	0.196%
29	12.463	1760	1764	1768	rVB2	128443	183995	2.71%	0.289%
30	12.504	1768	1771	1776	rBV	121108	143244	2.11%	0.225%
31	12.580	1781	1784	1787	rBV	1260465	1093254	16.08%	1.720%
32	12.686	1798	1802	1808	rBV2	560805	704791	10.36%	1.109%
33	12.810	1818	1823	1826	rBV	1181245	1163751	17.11%	1.831%
34	12.957	1844	1848	1852	rVB	4714777	4428140	65.12%	6.966%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119659.D
Acq On : 31 Mar 2020 18:34
Operator : MA/SJ
Sample : L2055-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6-(1-3)

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	13.139	1877	1879	1882	rVB	221225	201000	2.96%	0.316%
36	13.192	1886	1888	1889	rBV	124777	100101	1.47%	0.157%
37	13.245	1894	1897	1900	rVV2	187423	176899	2.60%	0.278%
38	13.339	1911	1913	1915	rVB	126257	88304	1.30%	0.139%
39	13.368	1916	1918	1921	rBV	112486	91706	1.35%	0.144%
40	13.539	1944	1947	1950	rBV2	177720	160817	2.37%	0.253%
41	13.868	2000	2003	2012	rVB2	683642	1022603	15.04%	1.609%
42	14.010	2023	2027	2030	rBV2	1748537	2262215	33.27%	3.559%
43	14.039	2030	2032	2035	rVB	580130	431433	6.34%	0.679%
44	14.186	2054	2057	2062	rVB2	268090	269424	3.96%	0.424%
45	14.492	2106	2109	2112	rBV3	455120	414209	6.09%	0.652%
46	14.798	2159	2161	2164	rBV	301846	286219	4.21%	0.450%
47	14.874	2172	2174	2178	rVB	433546	386206	5.68%	0.608%
48	15.057	2201	2205	2214	rVB	685108	1352916	19.90%	2.128%
49	15.421	2264	2267	2270	rBV	492013	537188	7.90%	0.845%
50	15.486	2274	2278	2281	rBV	936194	1172049	17.24%	1.844%

Sum of corrected areas: 63566850

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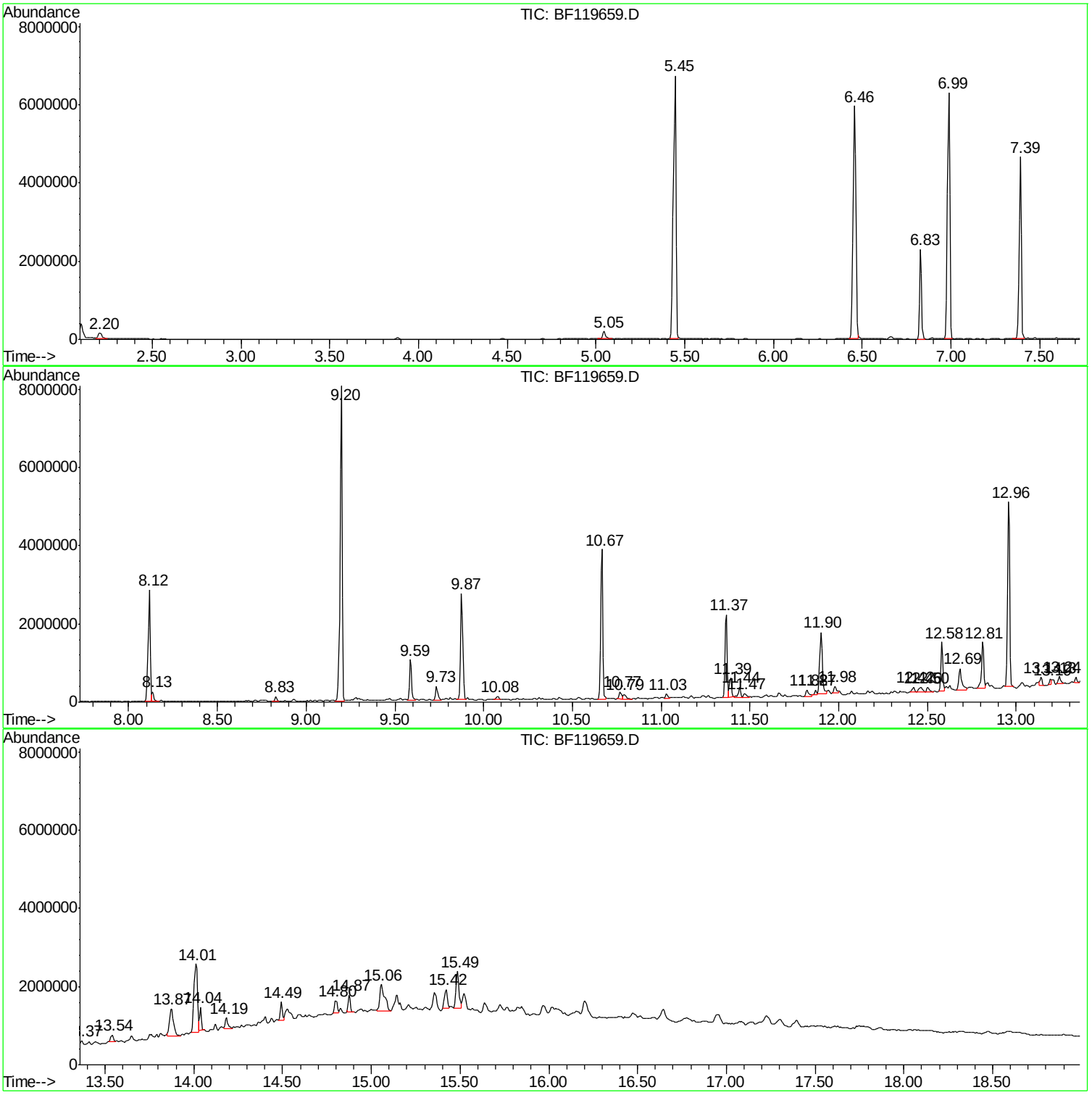
Sample : L2055-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-6-(1-3)

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119659.D
Acq On : 31 Mar 2020 18:34
Operator : MA/SJ
Sample : L2055-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6-(1-3)

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

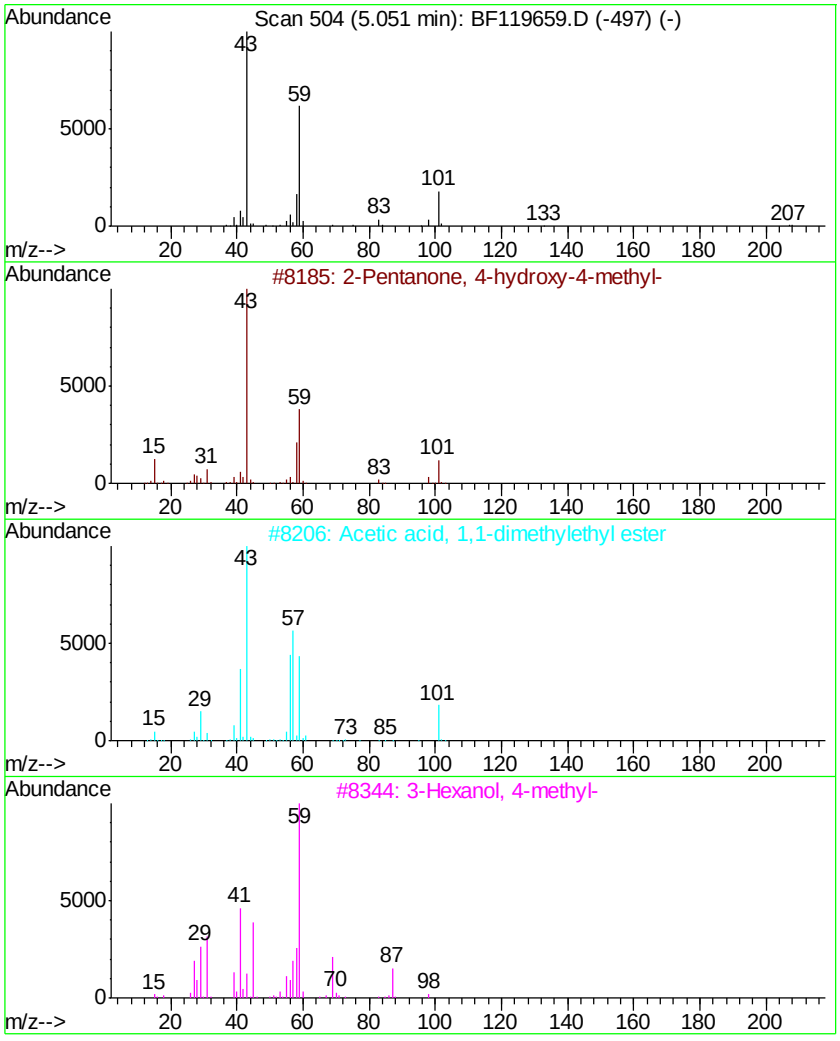
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

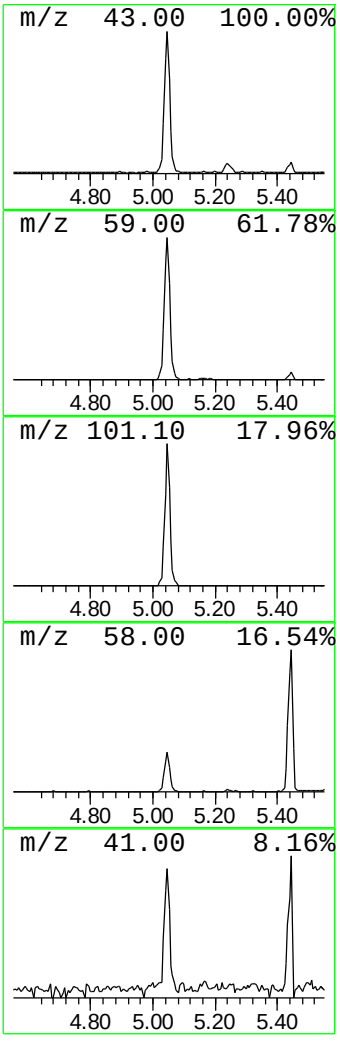
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	2.50 ng	232075	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119659.D
Acq On : 31 Mar 2020 18:34
Operator : MA/SJ
Sample : L2055-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6-(1-3)

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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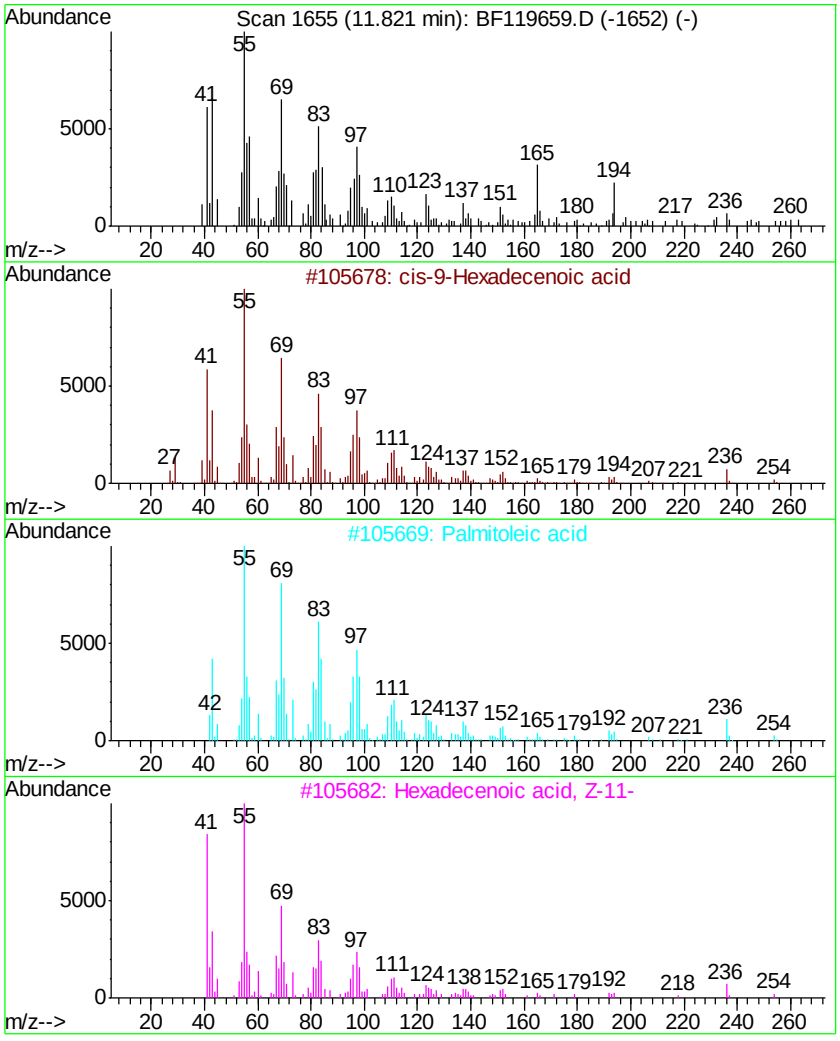
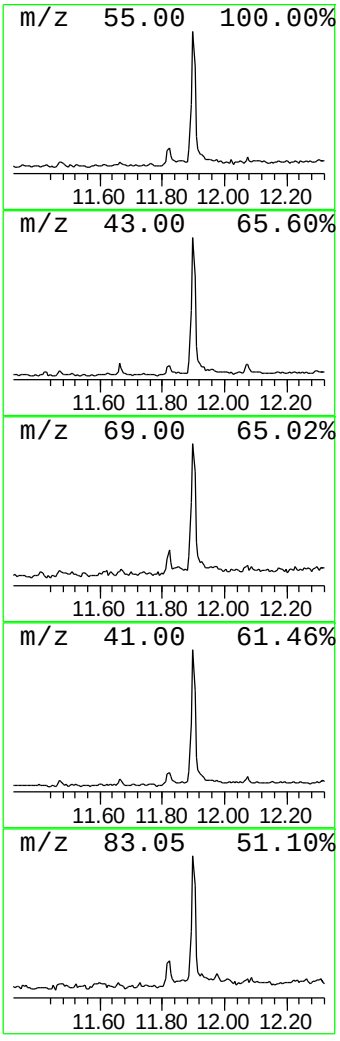
Peak Number 3 cis-9-Hexadecenoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	2.17 ng	209373	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	89
2	Palmitoleic acid	254	C16H30O2	000373-49-9	83
3	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	80
4	Z-7-Tetradecenoic acid	226	C14H26O2	1000130-98-4	72
5	E-3-Tetradecen-1-ol acetate	254	C16H30O2	1000130-81-1	59





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119659.D
Acq On : 31 Mar 2020 18:34
Operator : MA/SJ
Sample : L2055-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6-(1-3)

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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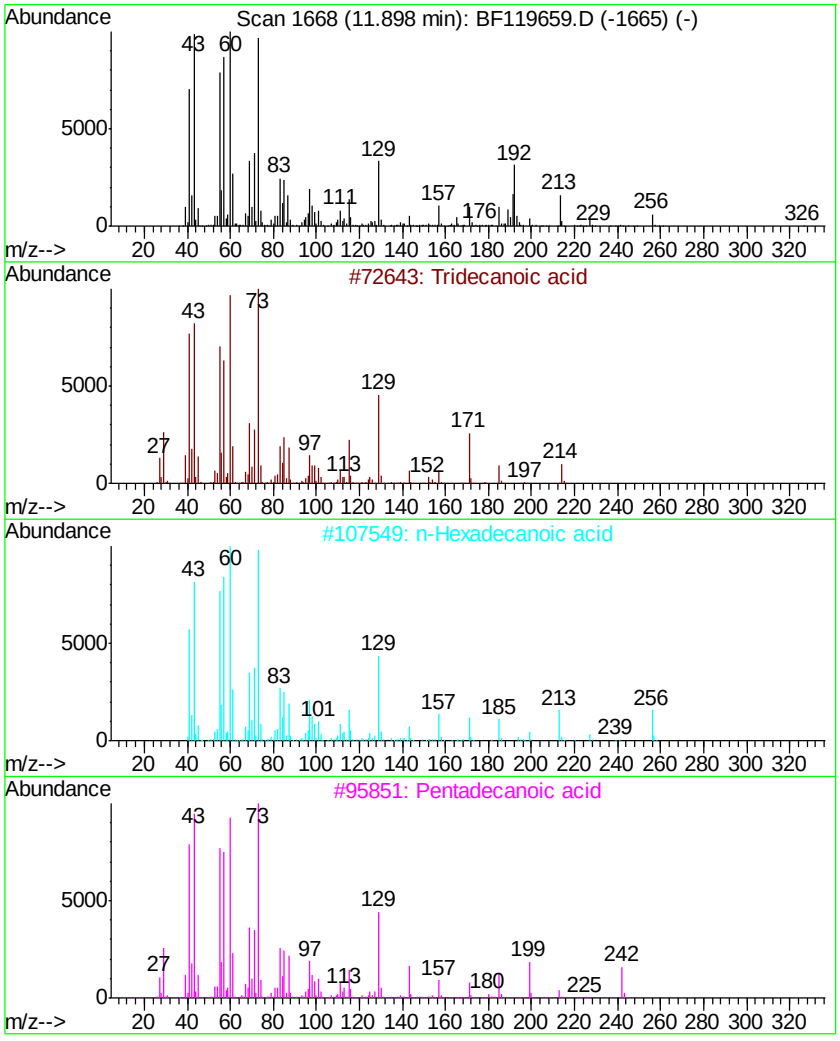
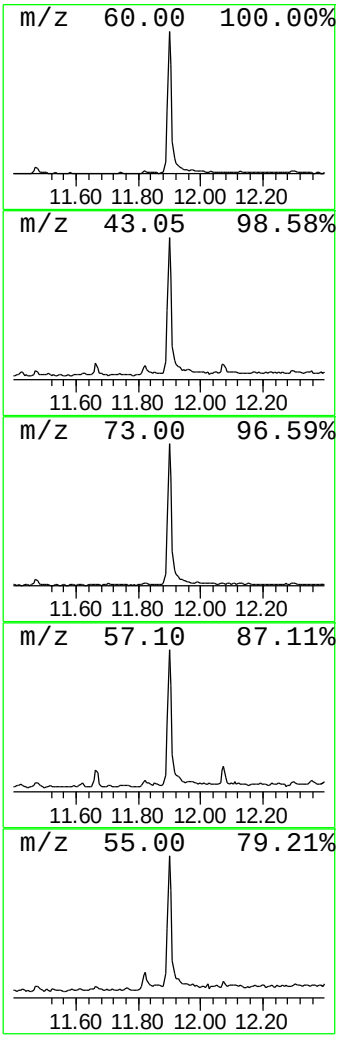
Peak Number 4 Tridecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	15.64 ng	1511080	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	93
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119659.D
Acq On : 31 Mar 2020 18:34
Operator : MA/SJ
Sample : L2055-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6-(1-3)

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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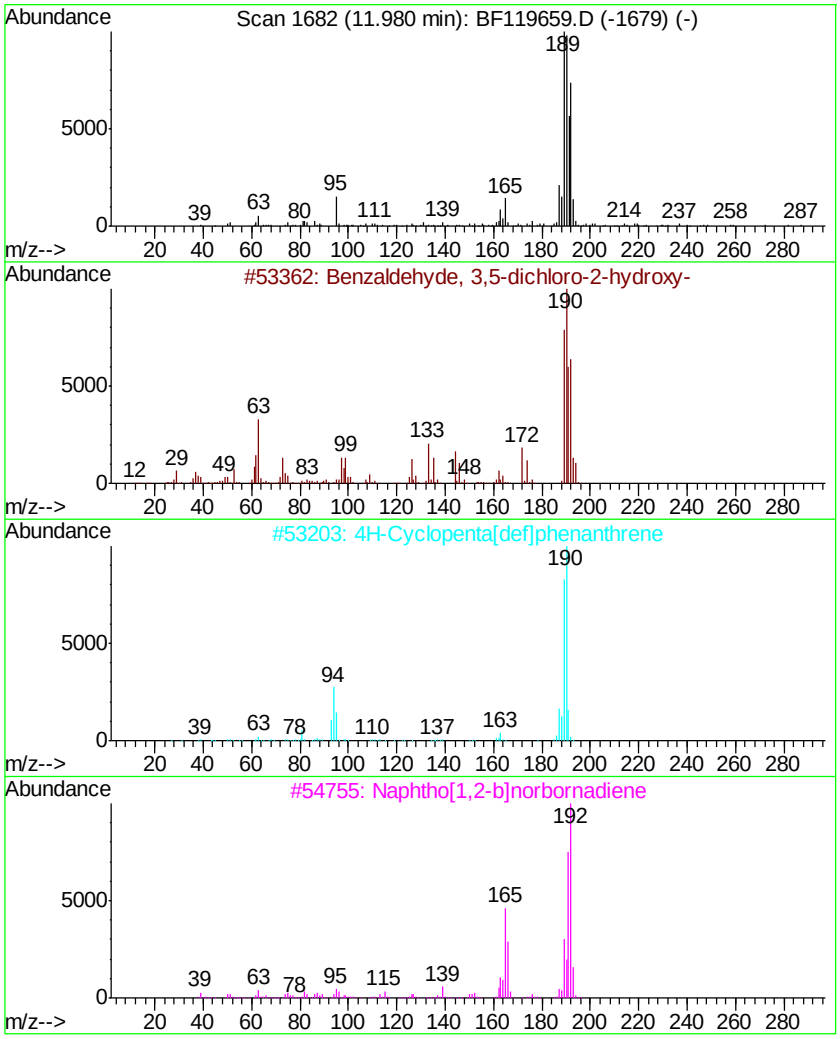
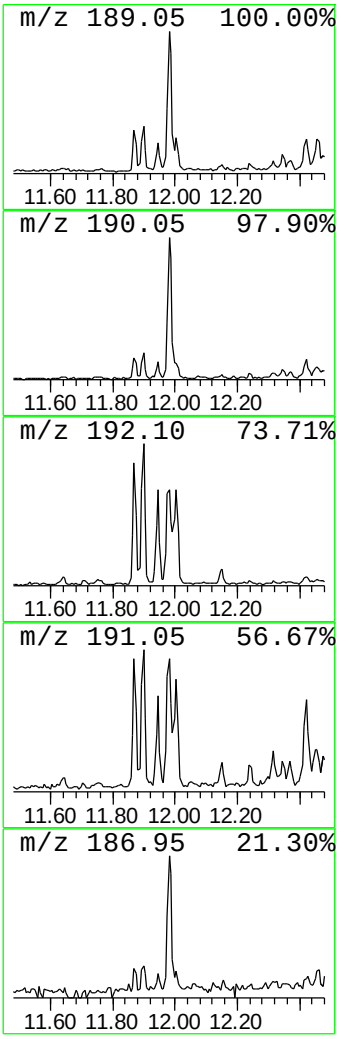
Peak Number 5 Benzaldehyde, 3,5-dichloro-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	2.08 ng	201102	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	80
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	53
3	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	41
4	Benzene, 1,1'-(2-cyclopropen-1-y...	192	C15H12	022825-21-4	38
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119659.D
Acq On : 31 Mar 2020 18:34
Operator : MA/SJ
Sample : L2055-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6-(1-3)

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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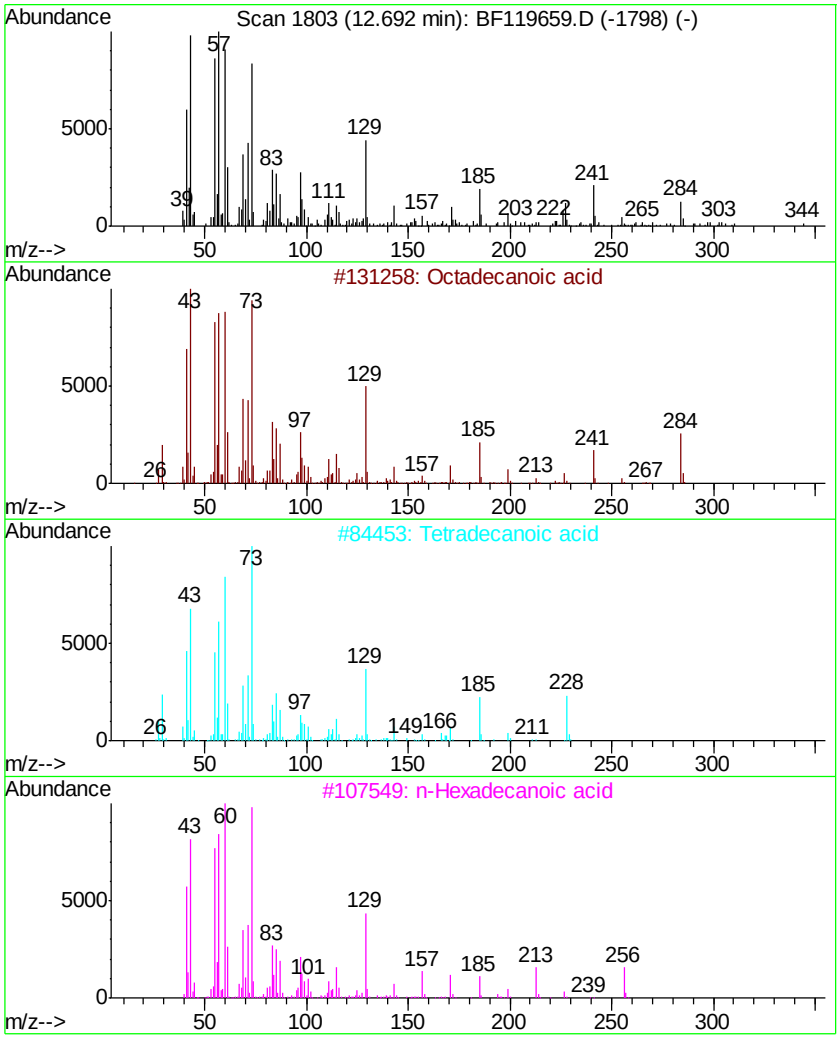
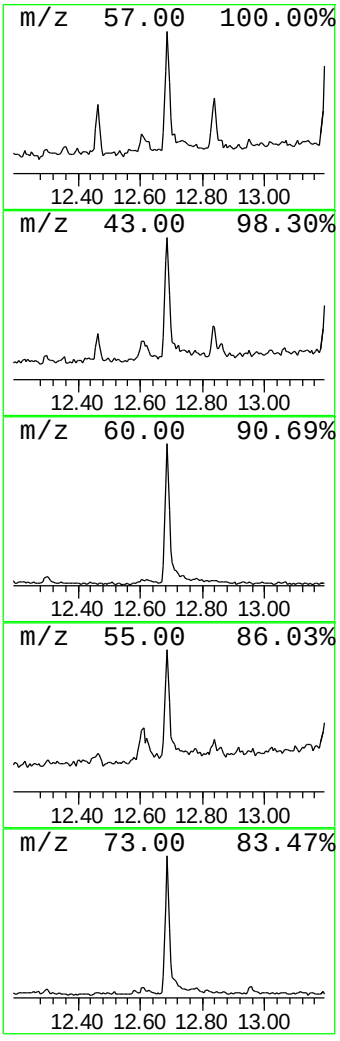
Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.69	7.29 ng	704791	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Dodecanoic acid	200	C12H24O2	000143-07-7	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119659.D
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Operator : MA/SJ
Sample : L2055-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6-(1-3)

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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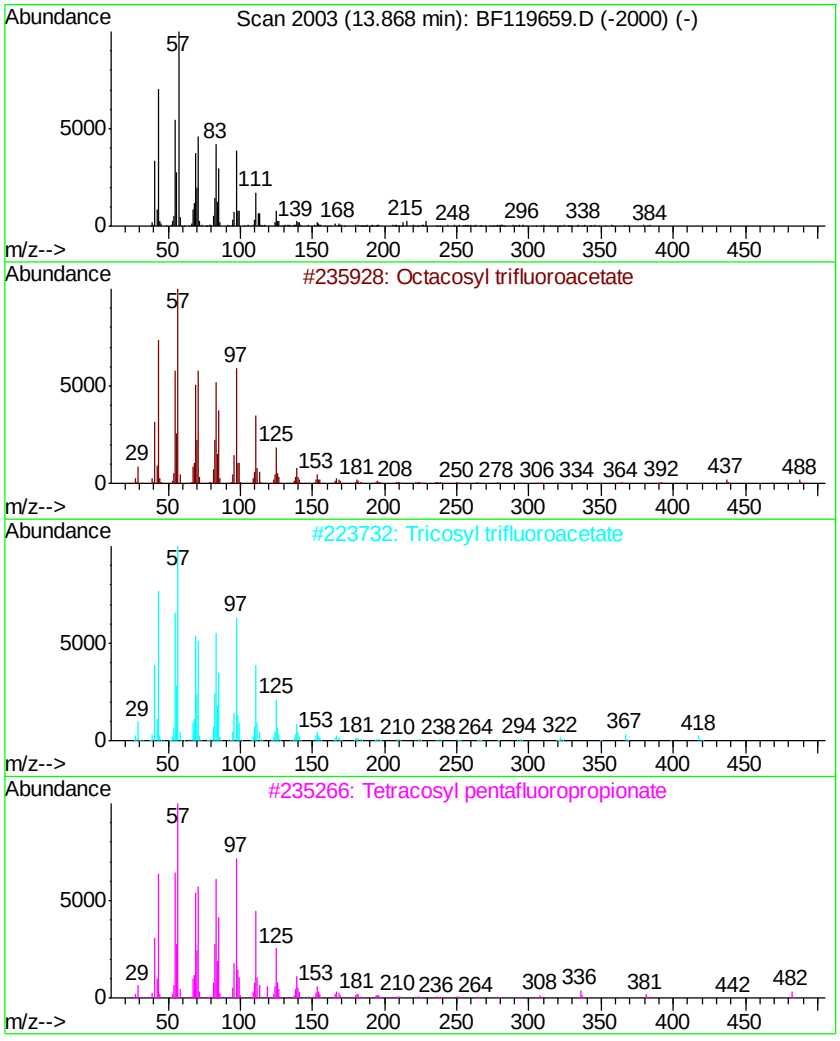
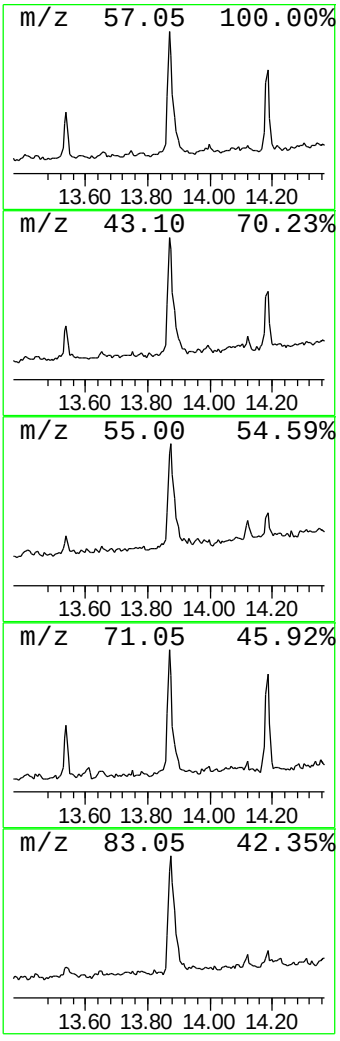
Peak Number 7 Octacosyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	9.04 ng	1022600	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
3	Tetracosyl pentafluoropropionate	500	C27H49F5O2	1000351-81-3	91
4	Methoxyacetic acid, heptadecyl e...	328	C20H40O3	1000282-99-1	83
5	Cyclotetracosane	336	C24H48	000297-03-0	81





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Data File : BF119659.D
Acq On : 31 Mar 2020 18:34
Operator : MA/SJ
Sample : L2055-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6-(1-3)

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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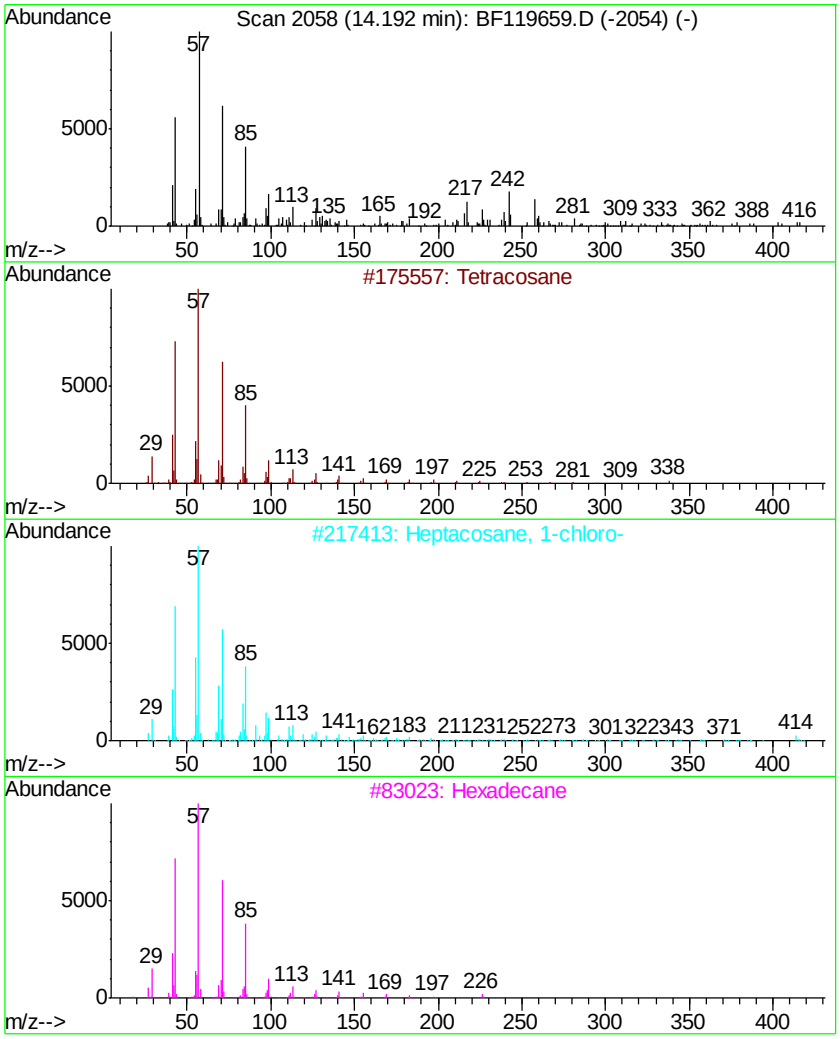
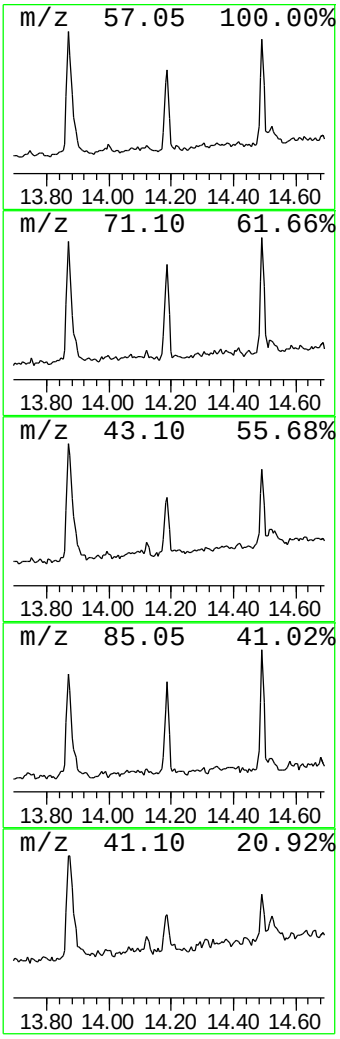
Peak Number 8 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	2.38 ng	269424	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	87
2	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	83
3	Hexadecane	226	C16H34	000544-76-3	80
4	Heneicosane	296	C21H44	000629-94-7	76
5	Docosane	310	C22H46	000629-97-0	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119659.D
Acq On : 31 Mar 2020 18:34
Operator : MA/SJ
Sample : L2055-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6-(1-3)

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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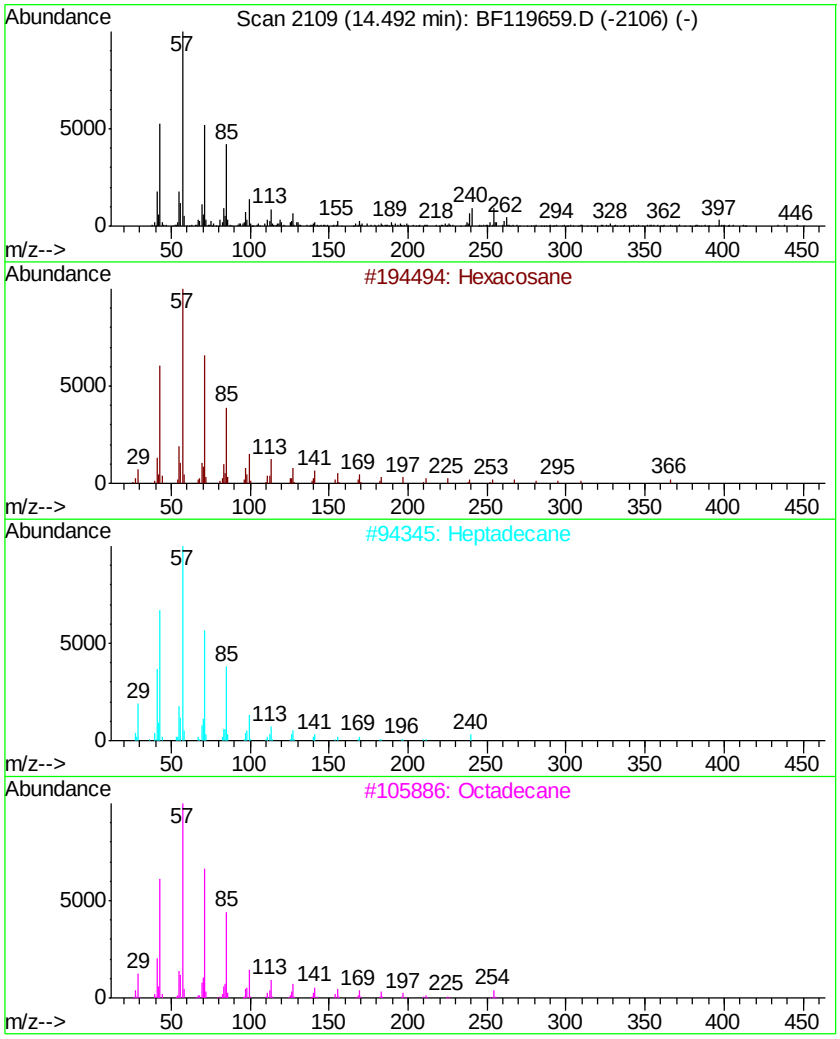
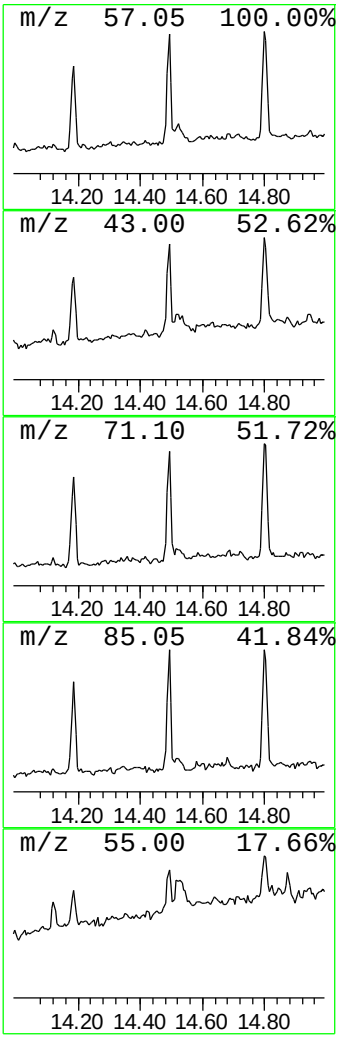
Peak Number 9 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.49	3.66 ng	414209	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Heptadecane	240	C17H36	000629-78-7	87
3	Octadecane	254	C18H38	000593-45-3	83
4	Eicosane, 9-octyl-	394	C28H58	013475-77-9	76
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	68





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119659.D
Acq On : 31 Mar 2020 18:34
Operator : MA/SJ
Sample : L2055-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6-(1-3)

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

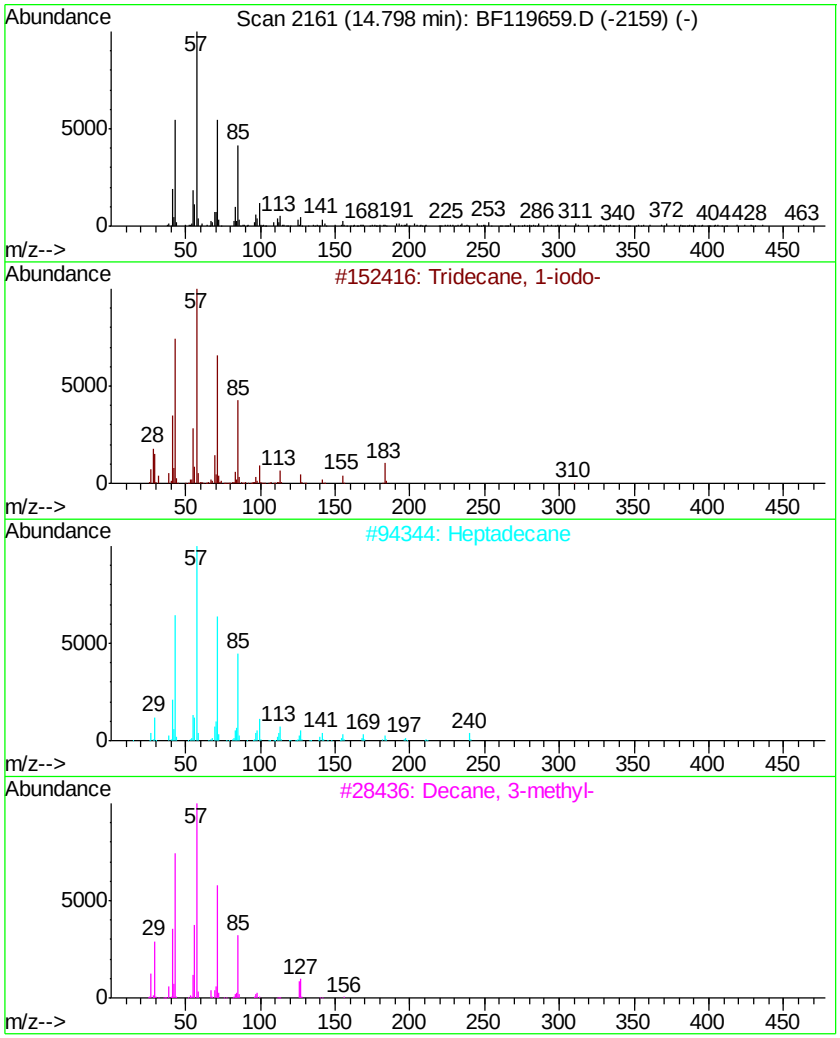
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

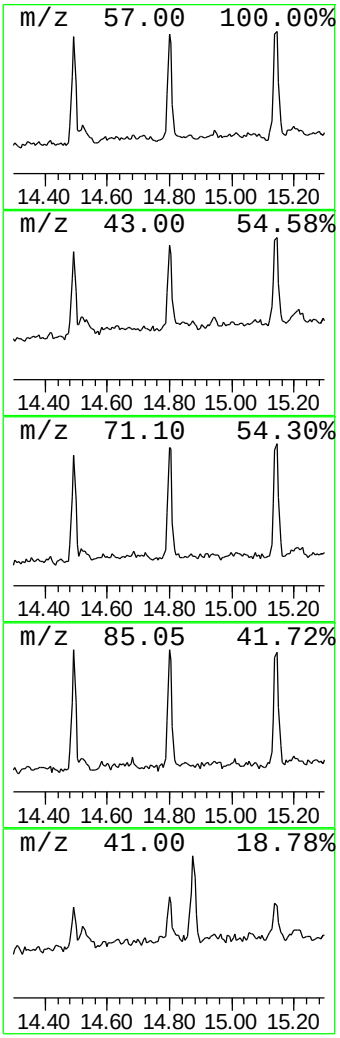
****

Peak Number 10 Tridecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	4.88 ng	286219	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
2	Heptadecane	240	C17H36	000629-78-7	80
3	Decane, 3-methyl-	156	C11H24	013151-34-3	72
4	Heptacosane	380	C27H56	000593-49-7	58
5	Pentadecane	212	C15H32	000629-62-9	53





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF033120\
Data File : BF119659.D
Acq On : 31 Mar 2020 18:34
Operator : MA/SJ
Sample : L2055-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6-(1-3)

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

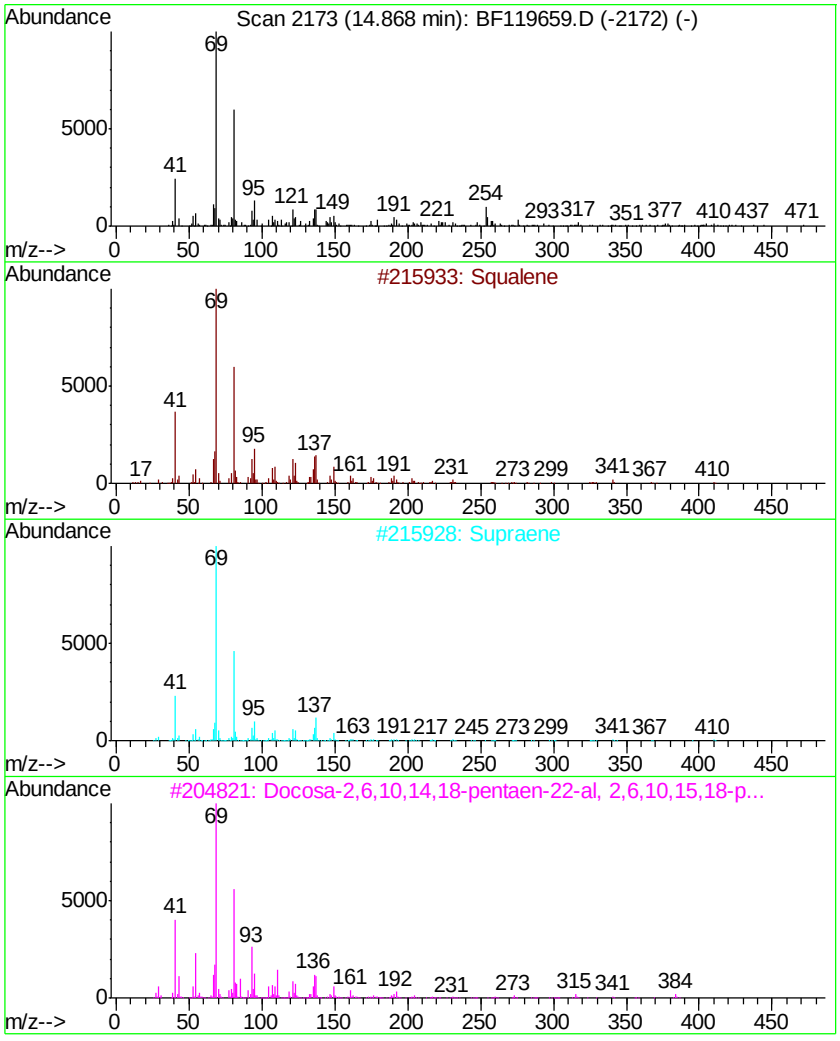
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

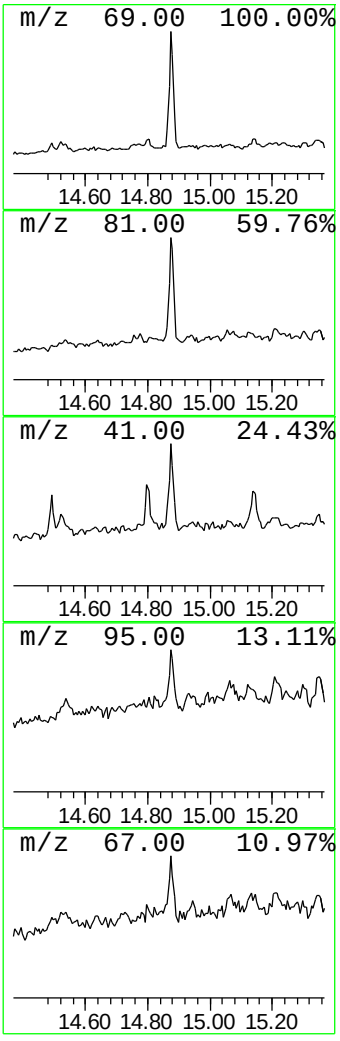
****

Peak Number 11 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	6.59 ng	386206	Perylene-d12	15.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	Supraene	410	C30H50	007683-64-9	64
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	64
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59
5	Farnesol isomer a	222	C15H26O	1000108-92-4	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF033120\
Data File : BF119659.D
Acq On : 31 Mar 2020 18:34
Operator : MA/SJ
Sample : L2055-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-6-(1-3)

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
2-Pentanone, 4-hy...	5.05	2.5	ng	232075	1	6.83	1854080	20.0
cis-9-Hexadecenoi...	11.82	2.2	ng	209373	4	11.37	1932800	20.0
Tridecanoic acid	11.90	15.6	ng	1511080	4	11.37	1932800	20.0
Benzaldehyde, 3,5...	11.98	2.1	ng	201102	4	11.37	1932800	20.0
Octadecanoic acid	12.69	7.3	ng	704791	4	11.37	1932800	20.0
Octacosyl trifluo...	13.87	9.0	ng	1022600	5	14.02	2262220	20.0
Tetracosane	14.19	2.4	ng	269424	5	14.02	2262220	20.0
Hexacosane	14.49	3.7	ng	414209	5	14.02	2262220	20.0
Tridecane, 1-iodo-	14.80	4.9	ng	286219	6	15.49	1172050	20.0
Squalene	14.87	6.6	ng	386206	6	15.49	1172050	20.0