LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121065.D
Acq On : 28 Jul 2020 12:49
Operator : JU/CG
Sample : L3403-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-1

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-BF071620.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	5.004	494	496	507	rVB	50321	60130	1.42%	0.208%
2	5.422	563	567	579	rBV	1419813	1402595	33.16%	4.849%
3	6.439	736	740	752	rBV	921904	899757	21.27%	3.111%
4	6.639	771	774	782	rBV	46244	55677	1.32%	0.192%
5	6.810	799	803	807	rBV	1058179	846121	20.01%	2.925%
6	7.375	894	899	902	rBV	2178640	1924085	45.50%	6.652%
7	8.092	1017	1021	1025	rBV	1257345	1056299	24.98%	3.652%
8	9.169	1200	1204	1207	rBV	3218958	3052774	72.18%	10.555%
9	9.269	1219	1221	1227	rVB3	71163	90963	2.15%	0.314%
10	9.563	1267	1271	1284	rBV	762814	668167	15.80%	2.310%
11	9.663	1284	1288	1295	rVV5	27945	44763	1.06%	0.155%
12	9.845	1315	1319	1331	rBV	1342401	1280205	30.27%	4.426%
13	10.633	1448	1453	1463	rBV	2162429	2335090	55.21%	8.073%
14	10.763	1471	1475	1478	rBV	53640	58418	1.38%	0.202%
15	10.904	1495	1499	1502	rVB	100898	89737	2.12%	0.310%
16	11.186	1543	1547	1552	rBV4	26137	50592	1.20%	0.175%
17	11.333	1568	1572	1577	rBV	1456673	1419184	33.56%	4.907%
18	11.374	1577	1579	1584	rVB3	41586	61277	1.45%	0.212%
19	11.868	1654	1663	1674	rBV2	850154	1116781	26.41%	3.861%
20	11.951	1674	1677	1684	rVB3	34735	58448	1.38%	0.202%
21	12.145	1707	1710	1716	rVB	73923	80045	1.89%	0.277%
22	12.204	1717	1720	1723	rBV	72231	67953	1.61%	0.235%
23	12.310	1734	1738	1741	rBV	542835	514676	12.17%	1.779%
24	12.363	1744	1747	1752	rVV	111844	112992	2.67%	0.391%
25	12.404	1752	1754	1761	rVB	41430	50739	1.20%	0.175%
26	12.563	1777	1781	1787	rVB	114412	121312	2.87%	0.419%
27	12.645	1792	1795	1799	rBV	260185	271167	6.41%	0.938%
28	12.710	1804	1806	1809	rVB	56851	47889	1.13%	0.166%
29	12.921	1837	1842	1845	rBV	3943486	4229176	100.00%	14.622%
30	13.133	1875	1878	1882	rBV	57214	69791	1.65%	0.241%
31	13.386	1918	1921	1926	rVB	107112	108194	2.56%	0.374%
32	13.439	1927	1930	1934	rVV	102137	98468	2.33%	0.340%
33	13.486	1935	1938	1942	rVV3	36013	51798	1.22%	0.179%
34	13.527	1942	1945	1949	rVV	666959	641276	15.16%	2.217%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121065.D
Acq On : 28 Jul 2020 12:49
Operator : JU/CG
Sample : L3403-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-1

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-BF071620.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.563	1949	1951	1955	rVV	115979	107029	2.53%	0.370%
36	13.604	1956	1958	1965	rVB	63175	67970	1.61%	0.235%
37	13.762	1982	1985	1990	rVB	53803	51984	1.23%	0.180%
38	13.815	1991	1994	2002	rBV	1305919	1730110	40.91%	5.982%
39	13.874	2002	2004	2009	rVB	81936	90332	2.14%	0.312%
40	13.968	2016	2020	2026	rBV	1413992	1400267	33.11%	4.841%
41	14.457	2100	2103	2110	rVB3	104841	159707	3.78%	0.552%
42	14.610	2126	2129	2132	rVB	61082	54028	1.28%	0.187%
43	14.727	2146	2149	2156	rBV3	89148	120745	2.86%	0.417%
44	15.415	2261	2266	2285	rVB2	917168	1354391	32.02%	4.683%
45	15.868	2341	2343	2349	rVB3	32063	44429	1.05%	0.154%
46	15.933	2349	2354	2366	rBV2	200539	502311	11.88%	1.737%
47	16.398	2429	2433	2446	rVB	104868	203478	4.81%	0.704%

Sum of corrected areas: 28923320

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
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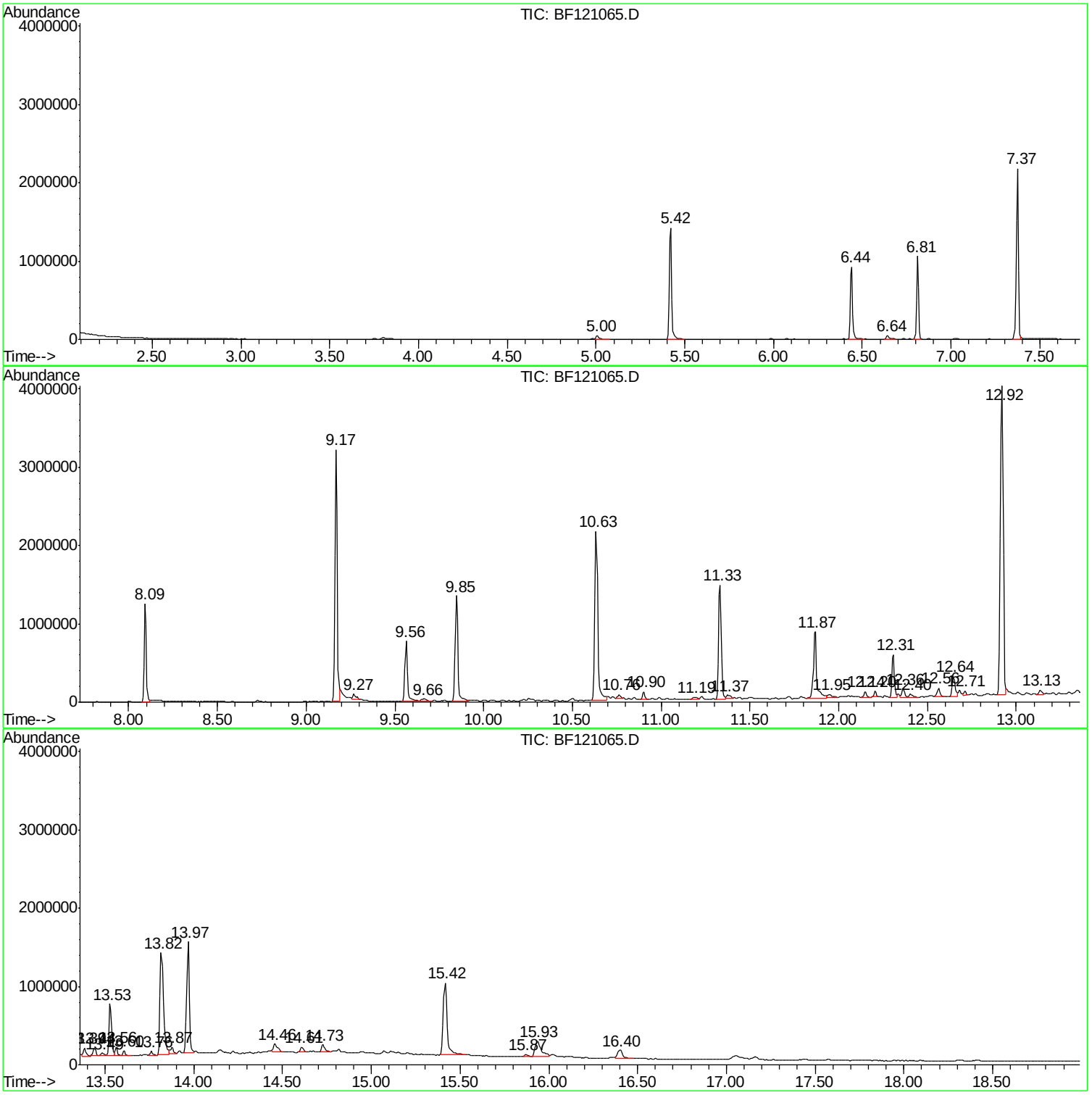
Instrument :
BNA_F
ClientSampleId :
W-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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\BF072820\
Data File : BF121065.D
Acq On : 28 Jul 2020 12:49
Operator : JU/CG
Sample : L3403-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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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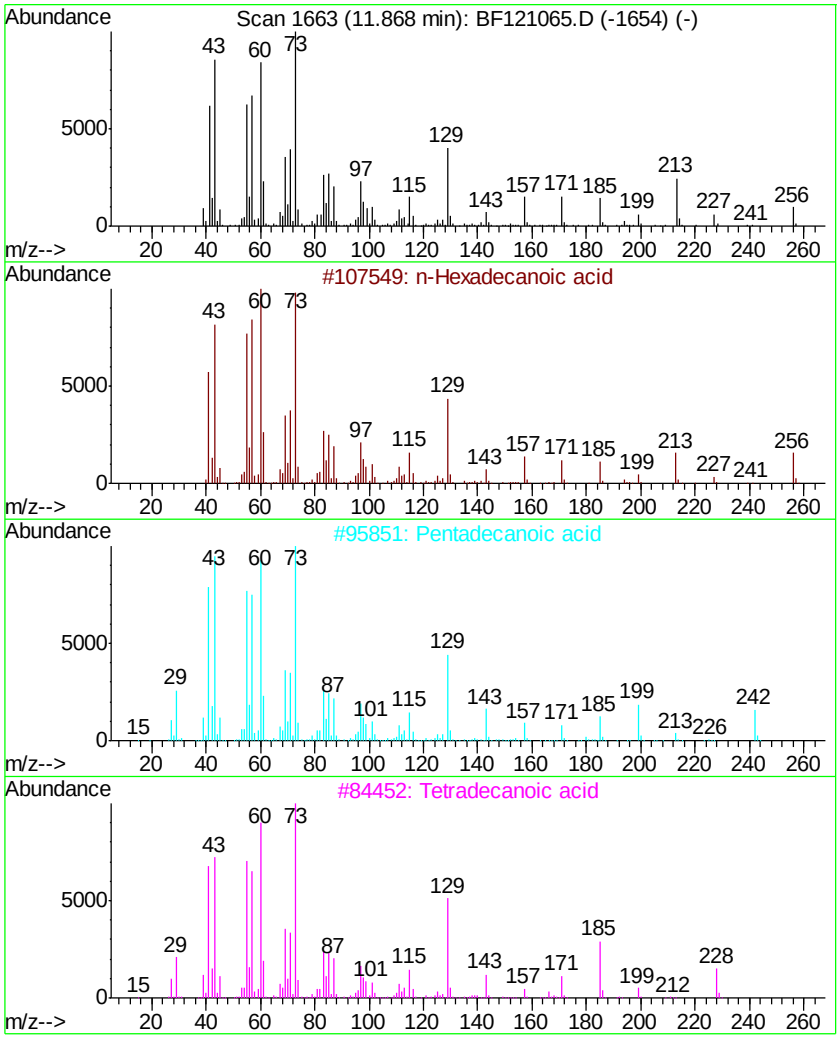
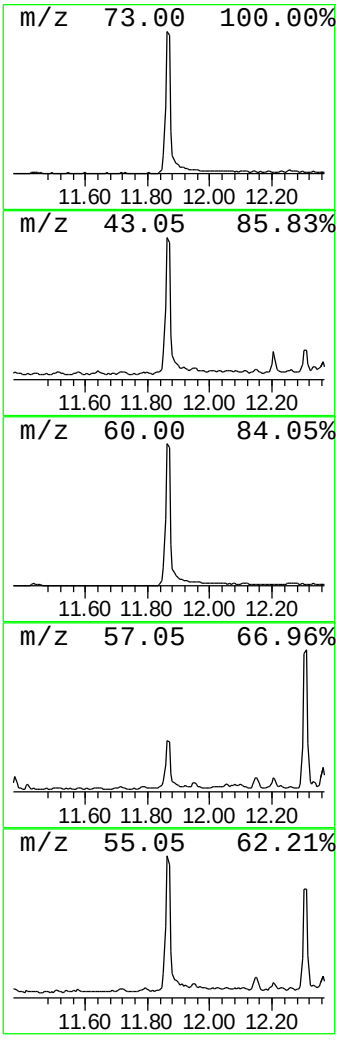
Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	15.74 ng	1116780	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	90
5	Dodecanoic acid	200	C12H24O2	000143-07-7	74





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121065.D
Acq On : 28 Jul 2020 12:49
Operator : JU/CG
Sample : L3403-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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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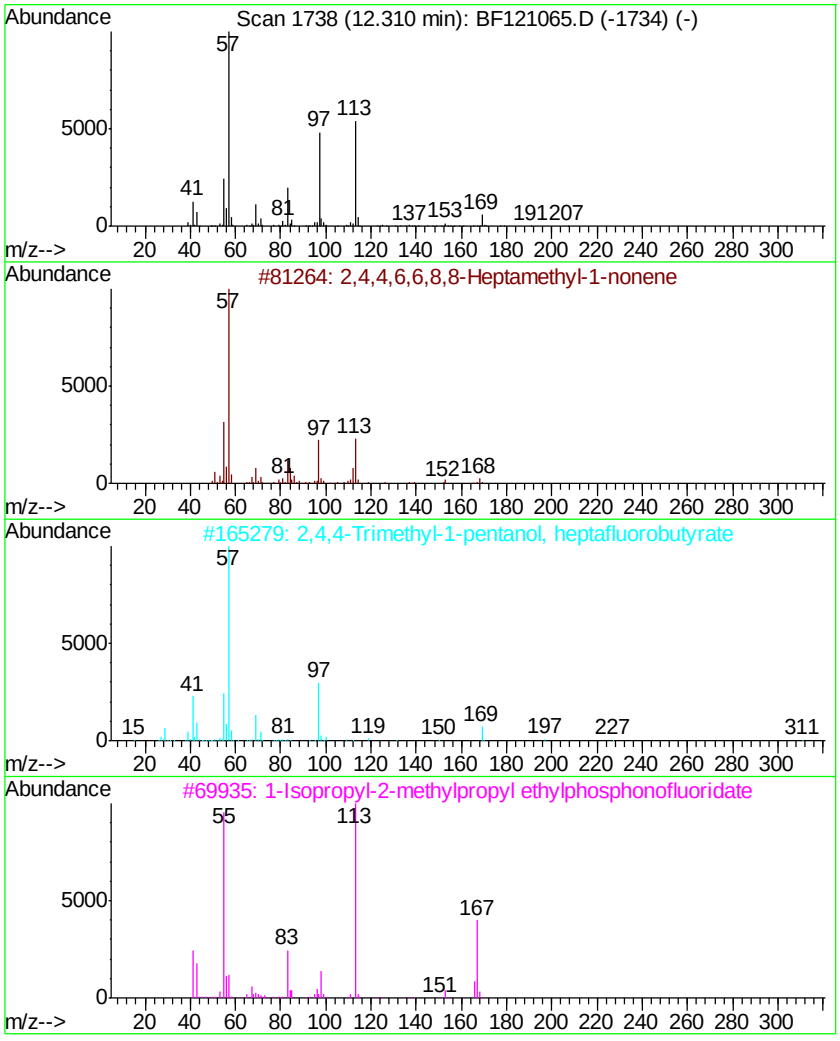
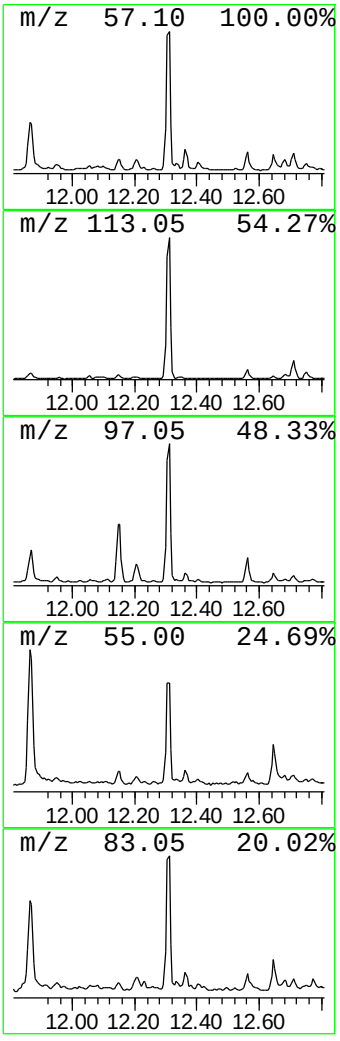
Peak Number 2 unknown12.31 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.31	7.25 ng	514676	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	37
2	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	35
3	1-Isopropyl-2-methylpropyl ethyl...	210	C9H20FO2P	1000298-33-2	32
4	Octane, 2-bromo-	192	C8H17Br	000557-35-7	32
5	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
Data File : BF121065.D
Acq On : 28 Jul 2020 12:49
Operator : JU/CG
Sample : L3403-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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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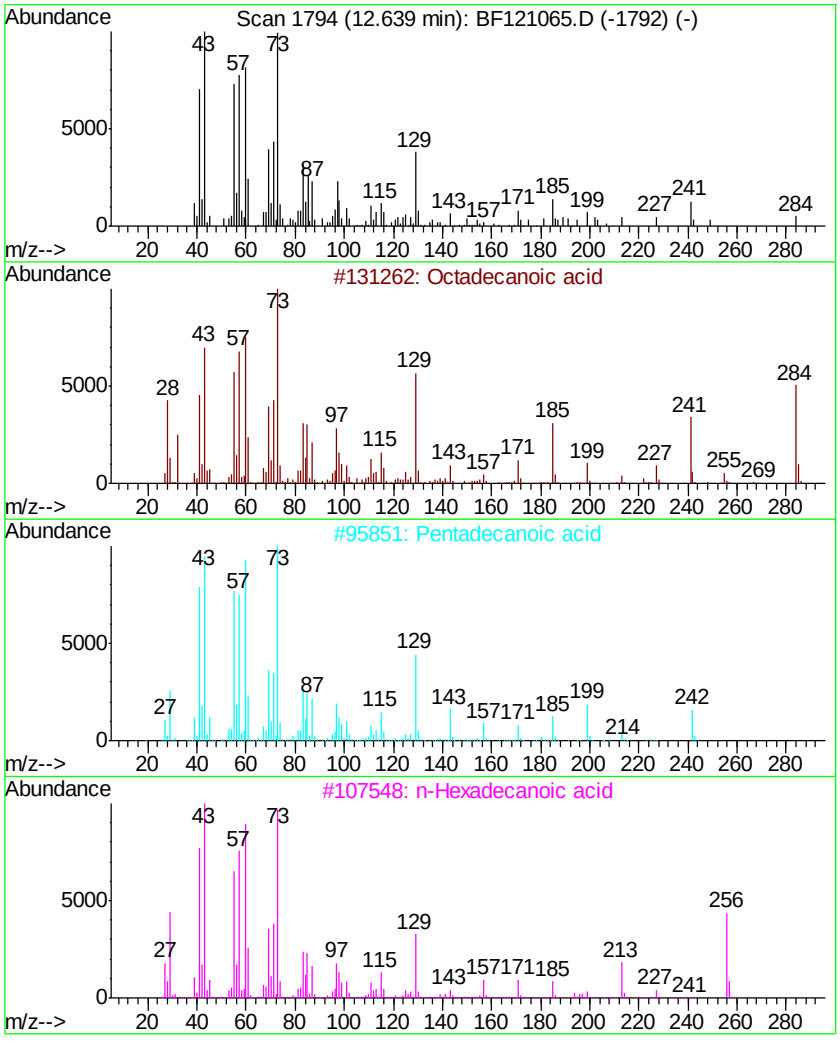
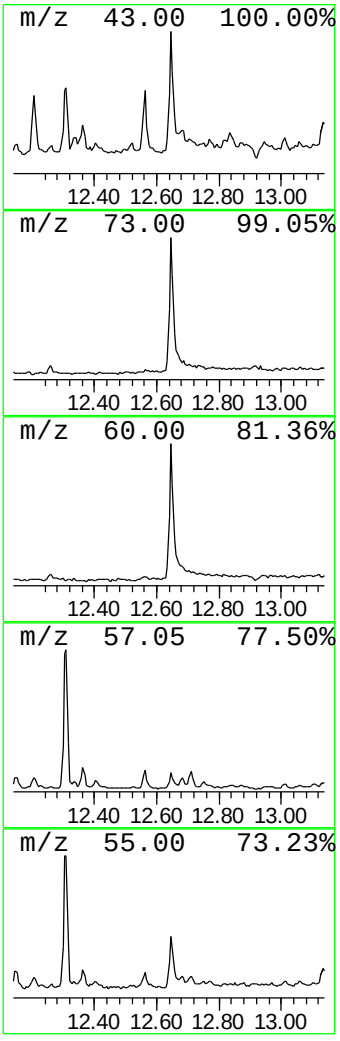
Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	3.82 ng	271167	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072820\
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Operator : JU/CG
Sample : L3403-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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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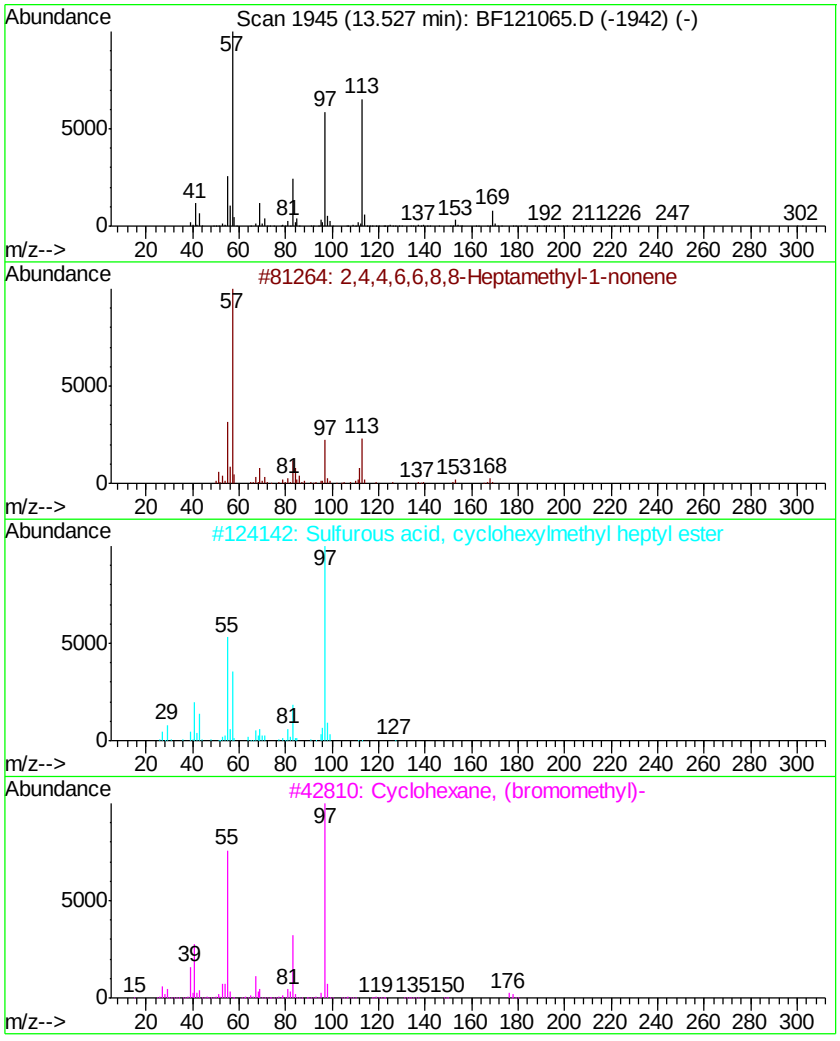
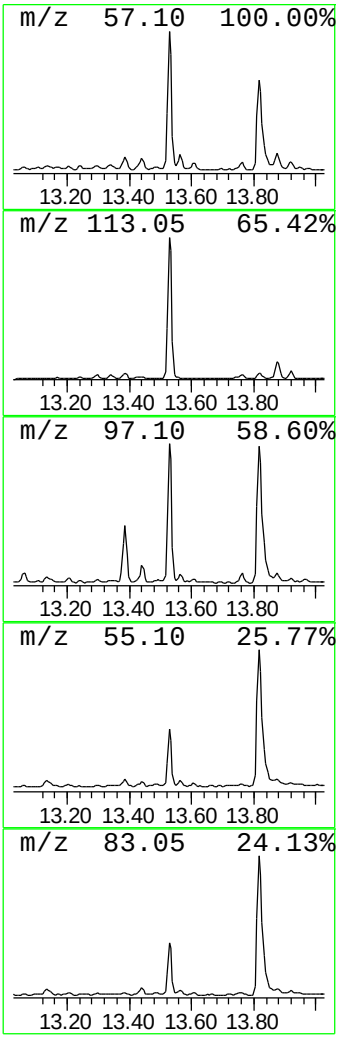
Peak Number 4 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.53	9.16 ng	641276	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	83
2	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	37
3	Cyclohexane, (bromomethyl)-	176	C7H13Br	002550-36-9	35
4	Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	25
5	Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	25





Library Search Compound Report

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Sample : L3403-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

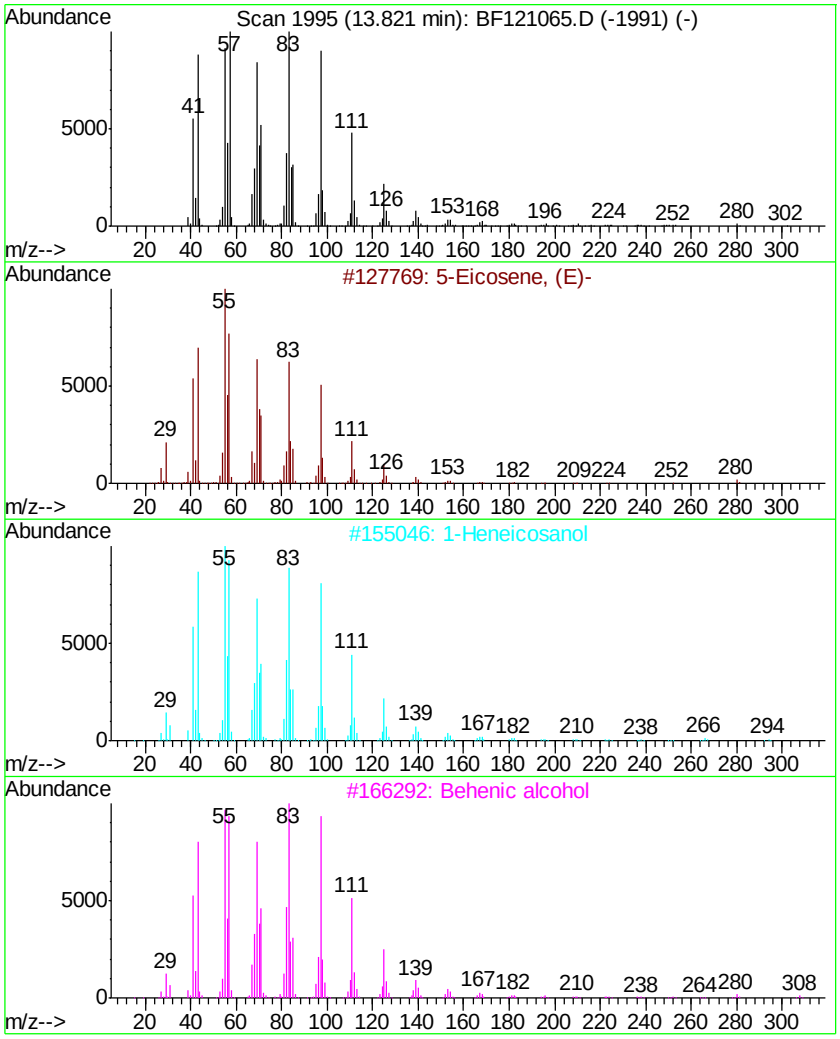
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

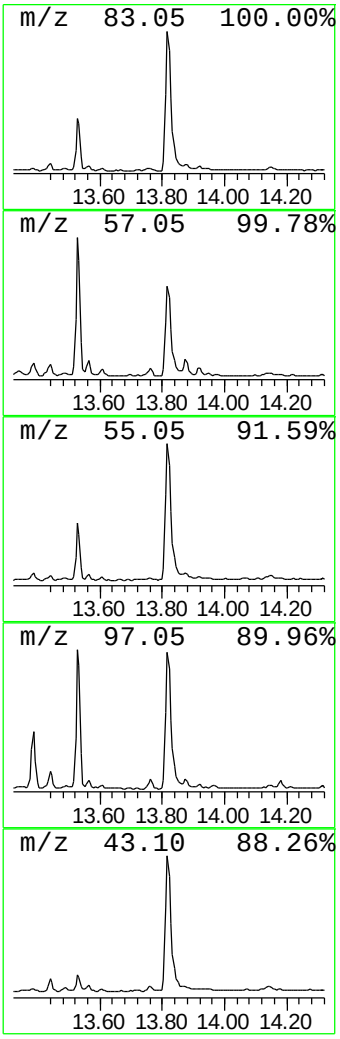
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	24.71 ng	1730110	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	94





Library Search Compound Report

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Data File : BF121065.D
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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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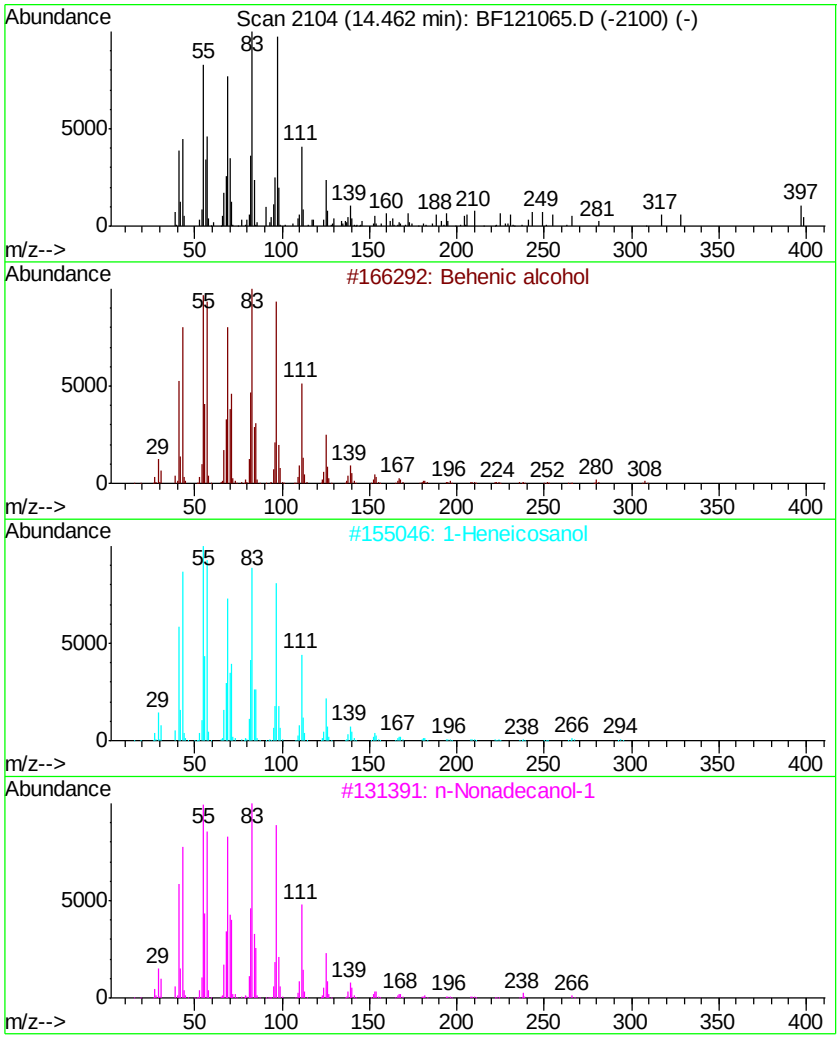
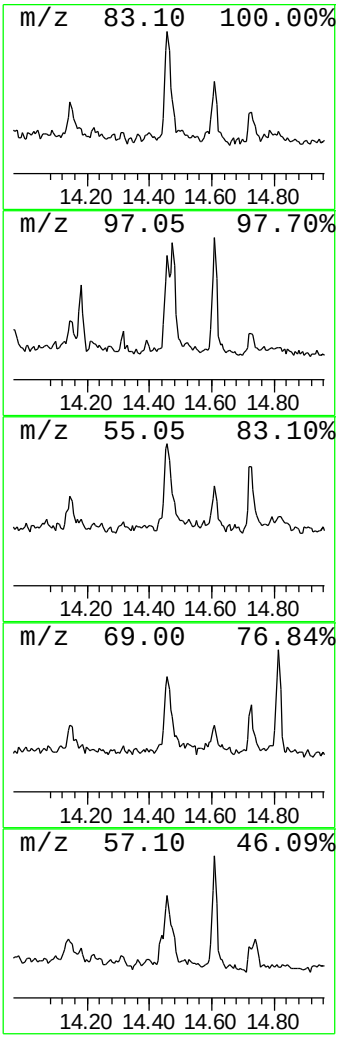
Peak Number 6 Behenic alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	2.28 ng	159707	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	90
2	1-Heneicosanol	312	C21H44O	015594-90-8	90
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	83
5	1-Octadecanol	270	C18H38O	000112-92-5	81





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Instrument : BNA_F
ClientSampleId : W-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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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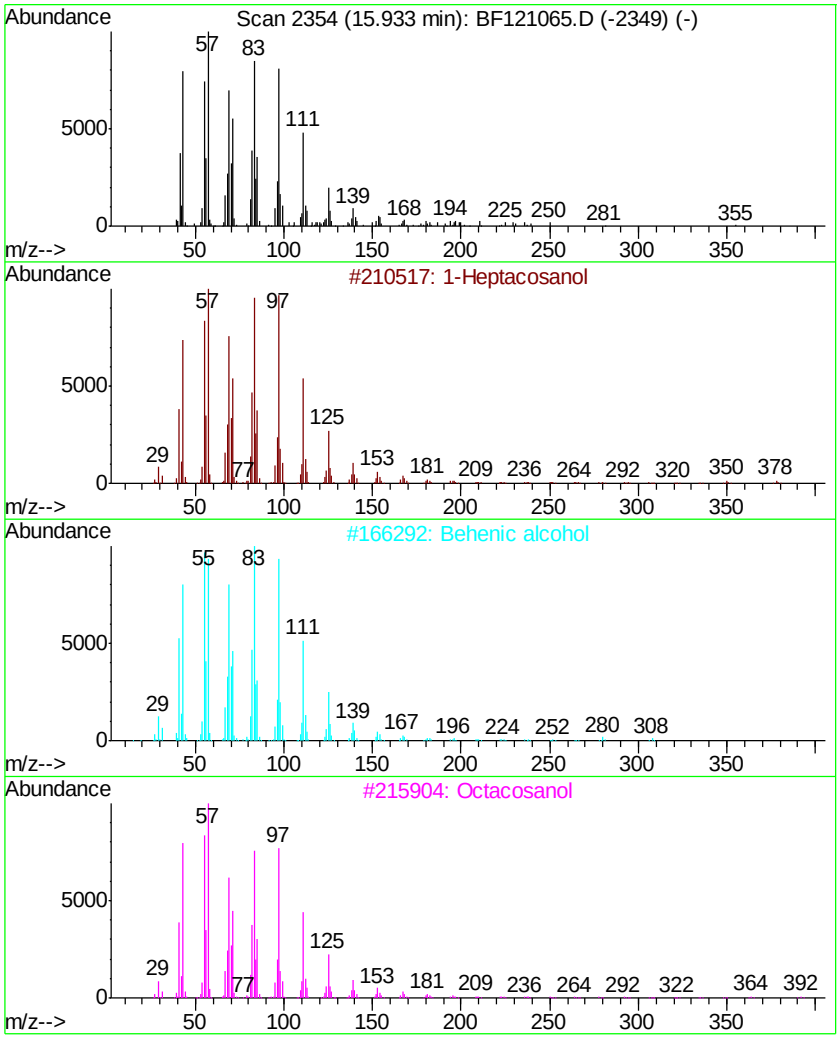
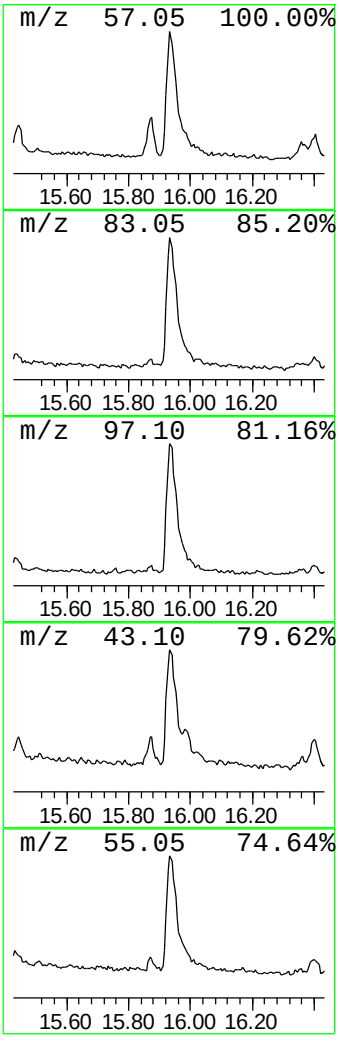
Peak Number 7 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	7.42 ng	502311	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	Octacosanol	410	C28H58O	000557-61-9	95
4	Triacontyl acetate	480	C32H64O2	041755-58-2	94
5	Heptacosyl acetate	438	C29H58O2	1000351-78-2	94





Library Search Compound Report

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Acq On : 28 Jul 2020 12:49
Operator : JU/CG
Sample : L3403-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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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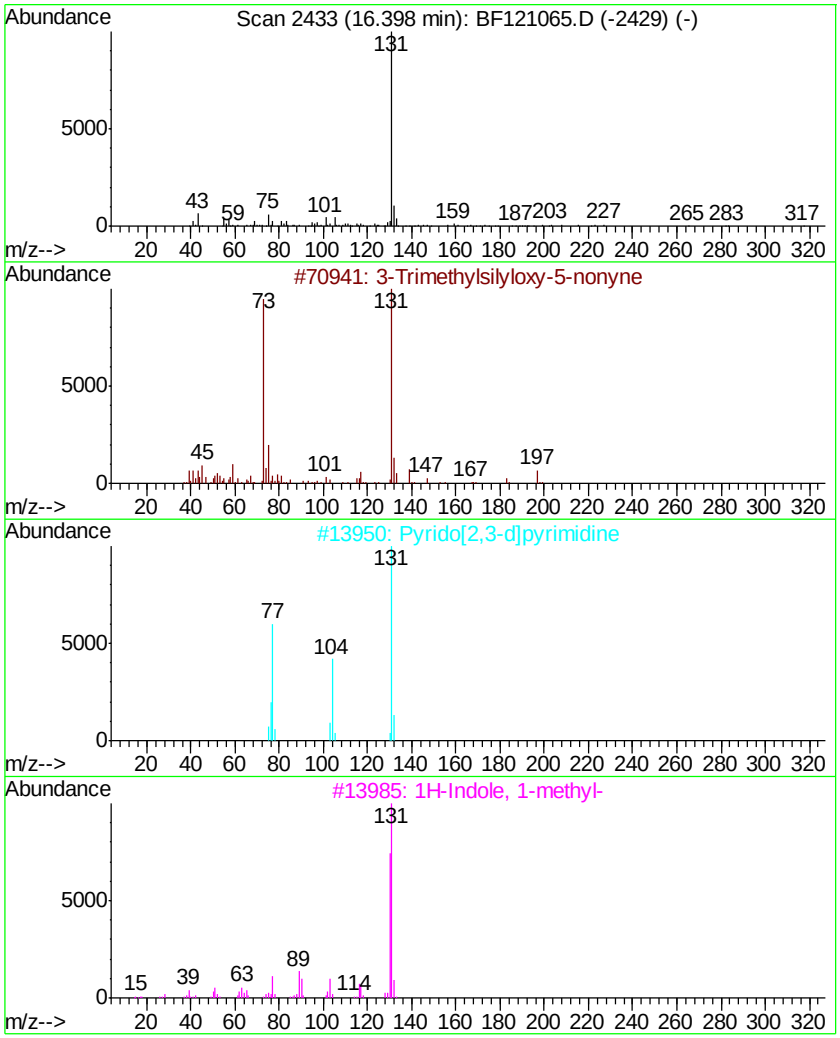
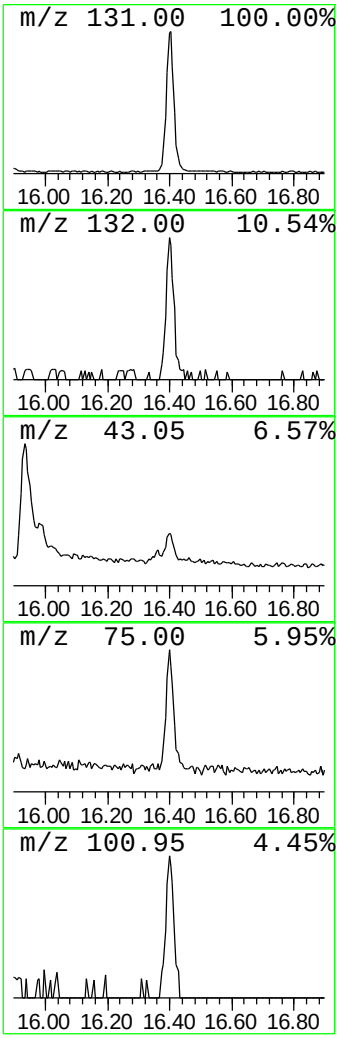
Peak Number 8 unknown16.40 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	3.00 ng	203478	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Trimethylsilyloxy-5-nonyne	212	C12H24OSi	1000245-72-4	43
2	Pyrido[2,3-d]pyrimidine	131	C7H5N3	000254-61-5	39
3	1H-Indole, 1-methyl-	131	C9H9N	000603-76-9	9
4	1H-Indole, 5-methyl-	131	C9H9N	000614-96-0	9
5	2,4(3H,5H)-Thiazoledione, 5-methyl-	131	C4H5NO2S	1000319-17-7	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072820\
Data File : BF121065.D
Acq On : 28 Jul 2020 12:49
Operator : JU/CG
Sample : L3403-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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 acid	11.87	15.7	ng	1116780	4	11.33	1419180	20.0
unknown12.31	12.31	7.3	ng	514676	4	11.33	1419180	20.0
Octadecanoic acid	12.64	3.8	ng	271167	4	11.33	1419180	20.0
2,4,4,6,6,8,8-Hep...	13.53	9.2	ng	641276	5	13.97	1400270	20.0
5-Eicosene, (E)-	13.82	24.7	ng	1730110	5	13.97	1400270	20.0
Behenic alcohol	14.46	2.3	ng	159707	5	13.97	1400270	20.0
1-Heptacosanol	15.93	7.4	ng	502311	6	15.42	1354390	20.0
unknown16.40	16.40	3.0	ng	203478	6	15.42	1354390	20.0