LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121020\
Data File : BF122651.D
Acq On : 10 Dec 2020 17:44
Operator : JU/CG
Sample : L4989-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-120920

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-BF120520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122651.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	7	10	16	rVB2	32596	40005	1.23%	0.122%
2	2.252	24	28	35	rVB	43683	59815	1.84%	0.183%
3	5.057	500	505	515	rBV	101567	131170	4.03%	0.401%
4	5.457	569	573	577	rBV	2897212	2991327	92.01%	9.140%
5	6.469	740	745	756	rBV	3018850	3251239	100.00%	9.934%
6	6.669	776	779	790	rBV	47181	66785	2.05%	0.204%
7	6.839	804	808	811	rBV	1303474	1139097	35.04%	3.480%
8	7.398	898	903	906	rBV	2116464	1944603	59.81%	5.941%
9	8.122	1021	1026	1043	rBV	1688781	1614979	49.67%	4.934%
10	9.198	1204	1209	1216	rBV	3263044	3109876	95.65%	9.502%
11	9.316	1224	1229	1233	rVB4	43068	51087	1.57%	0.156%
12	9.592	1268	1276	1284	rBV	237545	252186	7.76%	0.771%
13	9.875	1319	1324	1328	rBV	1976241	1868359	57.47%	5.709%
14	9.904	1328	1329	1340	rVB	122192	107730	3.31%	0.329%
15	10.080	1354	1359	1365	rBV	32392	37986	1.17%	0.116%
16	10.422	1414	1417	1423	rBV	74511	65390	2.01%	0.200%
17	10.663	1454	1458	1469	rBV	2270851	2169160	66.72%	6.628%
18	11.363	1572	1577	1579	rBV	2125629	1909207	58.72%	5.833%
19	11.386	1579	1581	1584	rVV	433331	377542	11.61%	1.154%
20	11.433	1587	1589	1593	rVB	117854	111487	3.43%	0.341%
21	11.592	1611	1616	1624	rBV	42673	56446	1.74%	0.172%
22	11.863	1658	1662	1664	rBV	39954	39383	1.21%	0.120%
23	11.892	1664	1667	1674	rVV	440398	467500	14.38%	1.428%
24	11.974	1678	1681	1684	rBV	81014	79613	2.45%	0.243%
25	12.574	1779	1783	1786	rBV	473850	445750	13.71%	1.362%
26	12.616	1786	1790	1792	rVV	96210	96537	2.97%	0.295%
27	12.680	1796	1801	1813	rVV	1038307	1196495	36.80%	3.656%
28	12.798	1816	1821	1827	rVB	407596	486491	14.96%	1.486%
29	12.945	1840	1846	1849	rBV	3428396	3045925	93.69%	9.306%
30	13.021	1854	1859	1863	rVB2	26807	40715	1.25%	0.124%
31	13.133	1875	1878	1881	rVB	74507	73838	2.27%	0.226%
32	13.198	1886	1889	1891	rVB	69569	56838	1.75%	0.174%
33	13.233	1891	1895	1897	rBV2	54184	52861	1.63%	0.162%
34	13.915	2003	2011	2018	rBV4	88598	310934	9.56%	0.950%
35	13.998	2019	2025	2028	rVV	1780946	1959080	60.26%	5.986%
36	14.021	2028	2029	2036	rVB	218788	188227	5.79%	0.575%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121020\
Data File : BF122651.D
Acq On : 10 Dec 2020 17:44
Operator : JU/CG
Sample : L4989-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-120920

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-BF120520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.104	2041	2043	2046	rVB	50488	39736	1.22%	0.121%
38	14.386	2087	2091	2095	rBV	31265	42428	1.30%	0.130%
39	14.468	2103	2105	2110	rVB3	31019	36913	1.14%	0.113%
40	14.533	2114	2116	2119	rVB2	42342	37882	1.17%	0.116%
41	14.845	2166	2169	2173	rBV	49727	59640	1.83%	0.182%
42	15.033	2197	2201	2205	rBV	166537	258672	7.96%	0.790%
43	15.110	2210	2214	2217	rVV	84596	105675	3.25%	0.323%
44	15.145	2217	2220	2224	rVB	33683	40314	1.24%	0.123%
45	15.333	2249	2252	2259	rVB	89564	125286	3.85%	0.383%
46	15.398	2259	2263	2268	rBV	112573	147235	4.53%	0.450%
47	15.462	2268	2274	2288	rVB	1069403	1497839	46.07%	4.576%
48	15.686	2309	2312	2317	rVB5	36170	52490	1.61%	0.160%
49	15.915	2347	2351	2357	rBV	52658	76176	2.34%	0.233%
50	16.415	2433	2436	2443	rVB3	25589	37528	1.15%	0.115%
51	16.909	2516	2520	2530	rVB3	42393	90260	2.78%	0.276%
52	17.351	2591	2595	2602	rVB	39025	70621	2.17%	0.216%
53	18.509	2785	2792	2803	rVB	38663	114843	3.53%	0.351%

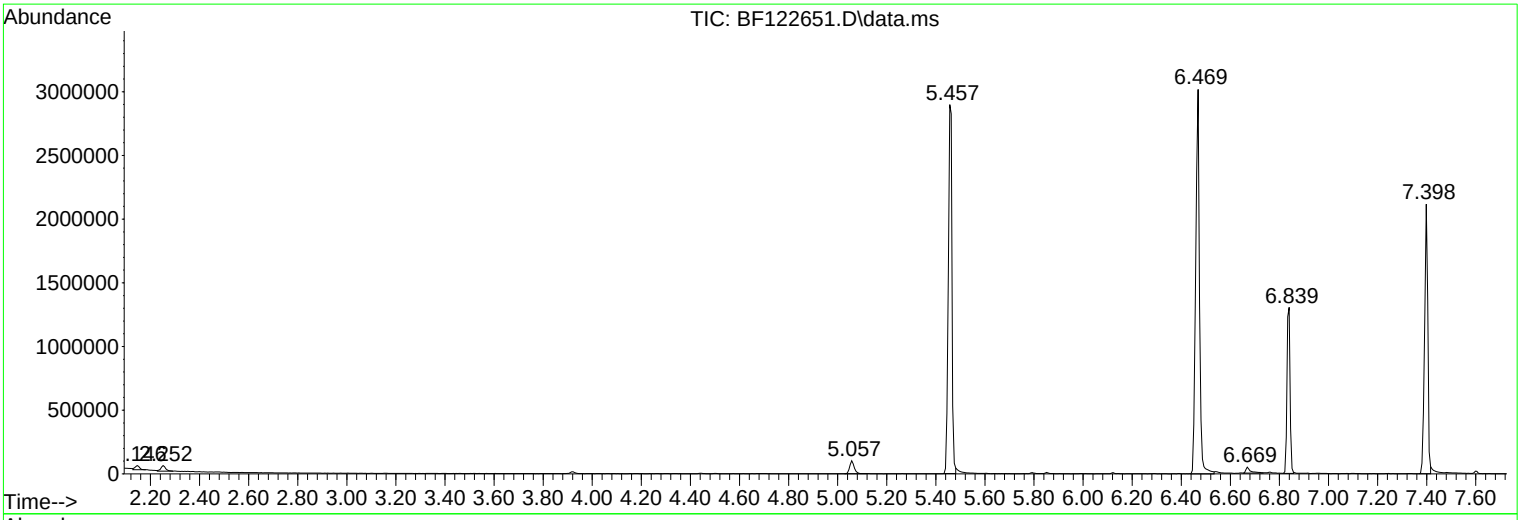
Sum of corrected areas: 32729201

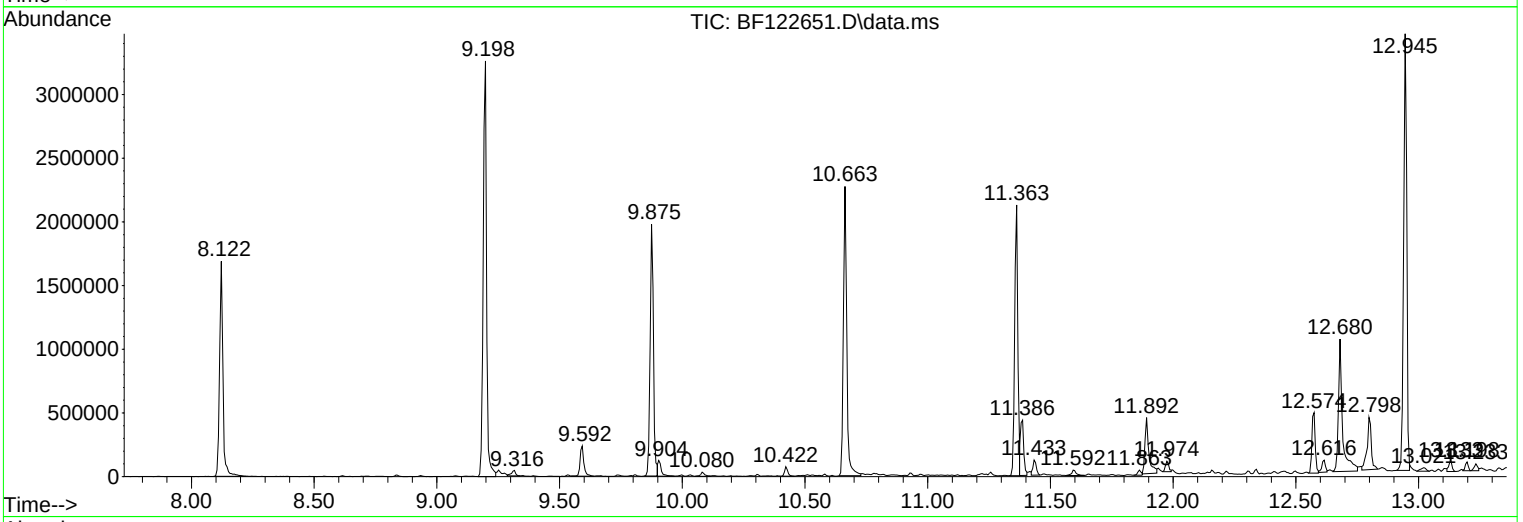
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121020\
Data File : BF122651.D
Acq On : 10 Dec 2020 17:44
Operator : JU/CG
Sample : L4989-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

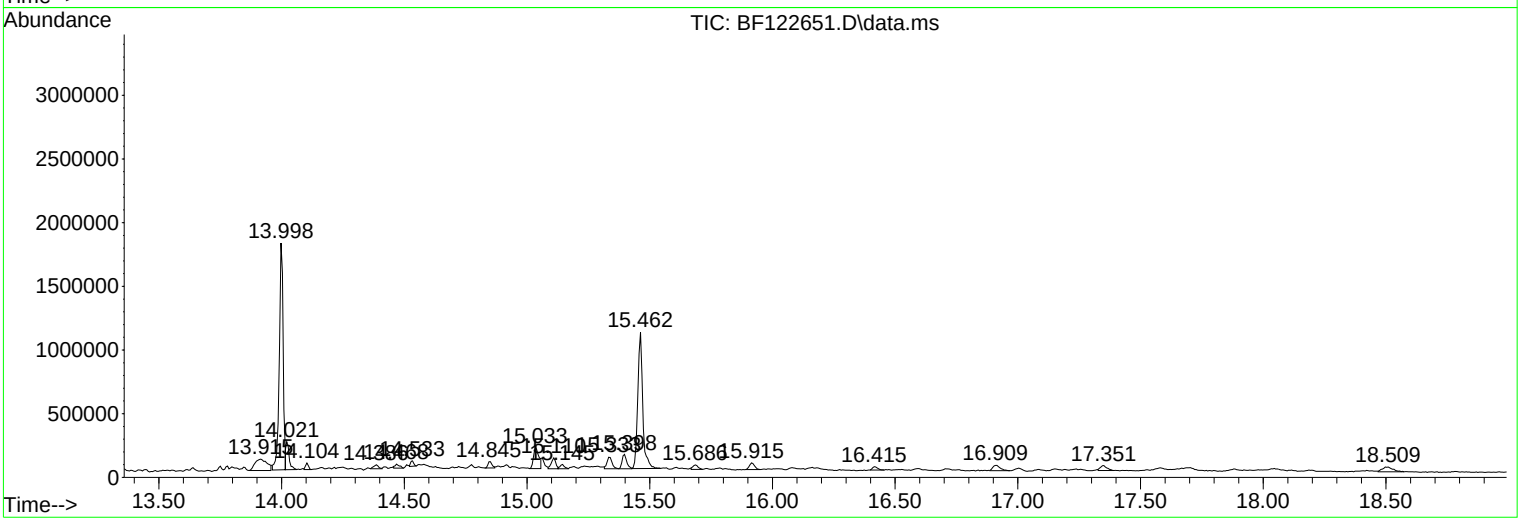
Instrument :
BNA_F
ClientSampleId :
BU-02-120920

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.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\BF121020\
Data File : BF122651.D
Acq On : 10 Dec 2020 17:44
Operator : JU/CG
Sample : L4989-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-120920

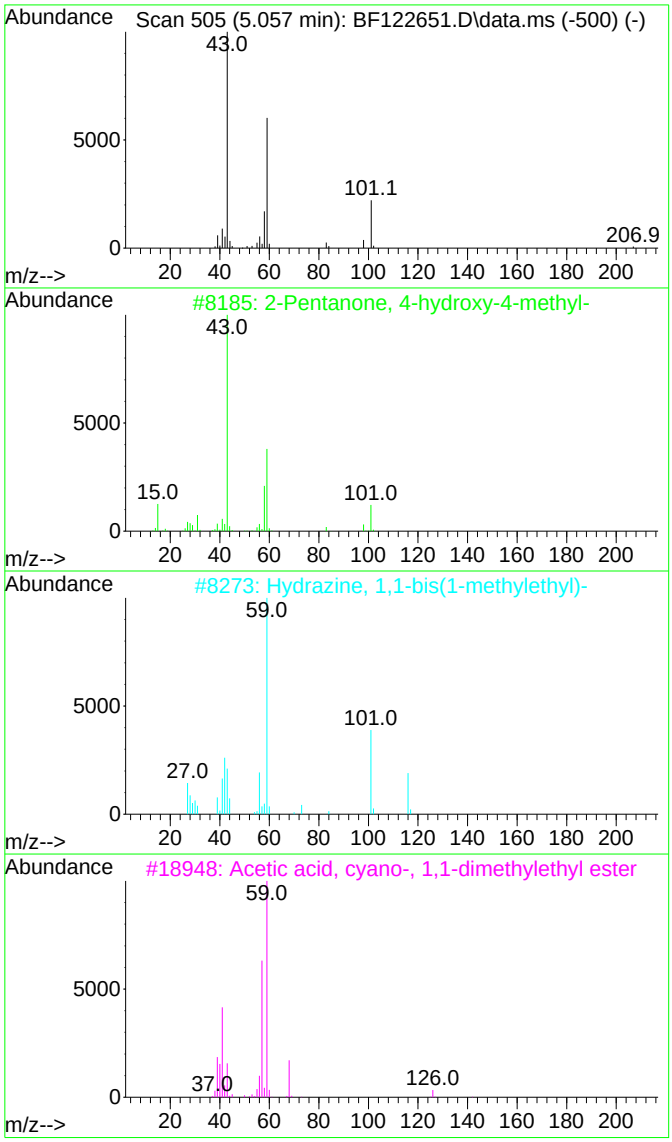
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

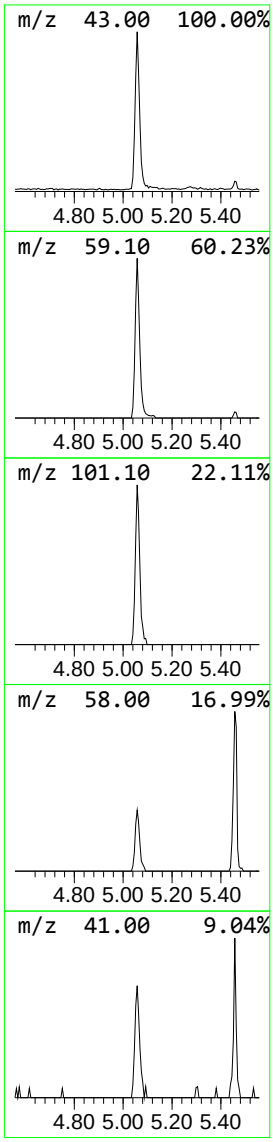
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	2.30 ng	131170	1,4-Dichlorobenzene-d4	6.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121020\
Data File : BF122651.D
Acq On : 10 Dec 2020 17:44
Operator : JU/CG
Sample : L4989-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-120920

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

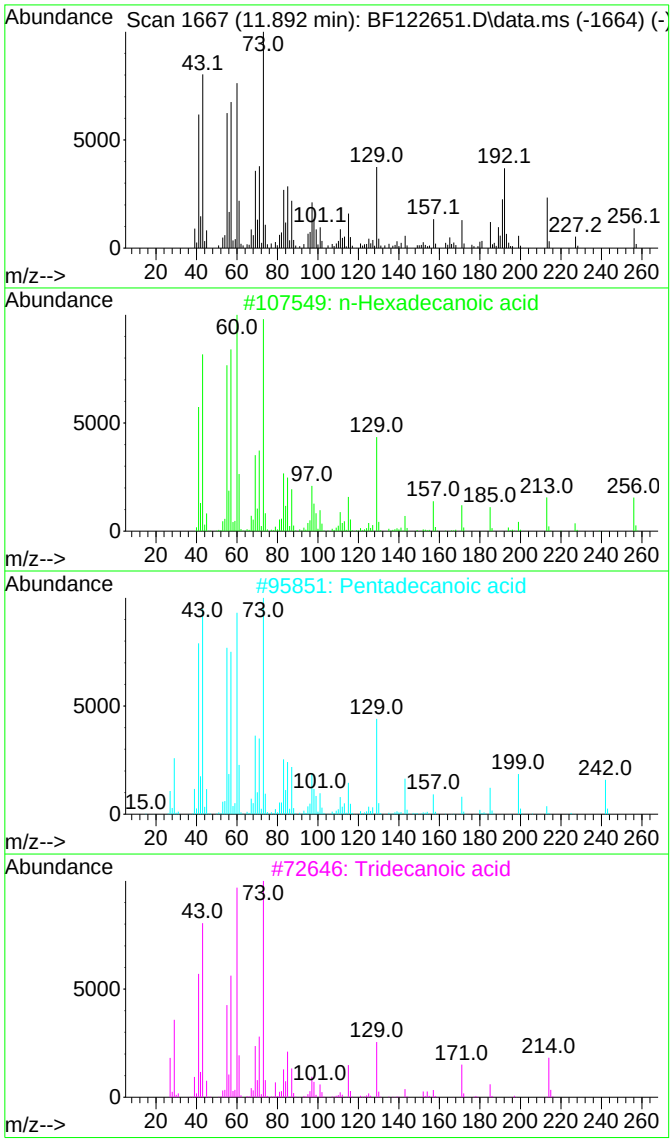
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

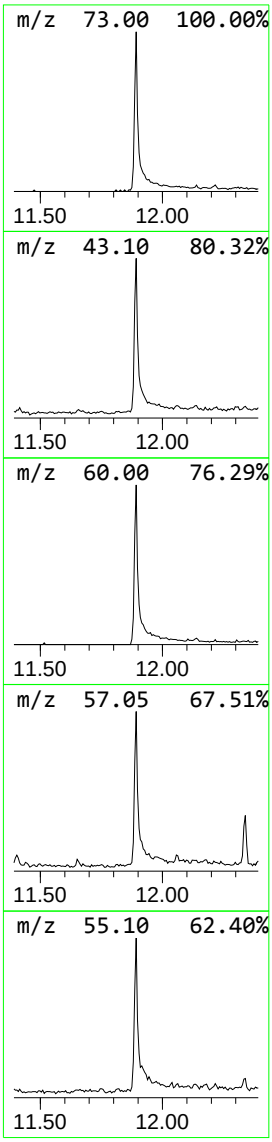
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	4.90 ng	467500	Phenanthrene-d10	11.363

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	89
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121020\
Data File : BF122651.D
Acq On : 10 Dec 2020 17:44
Operator : JU/CG
Sample : L4989-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-120920

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

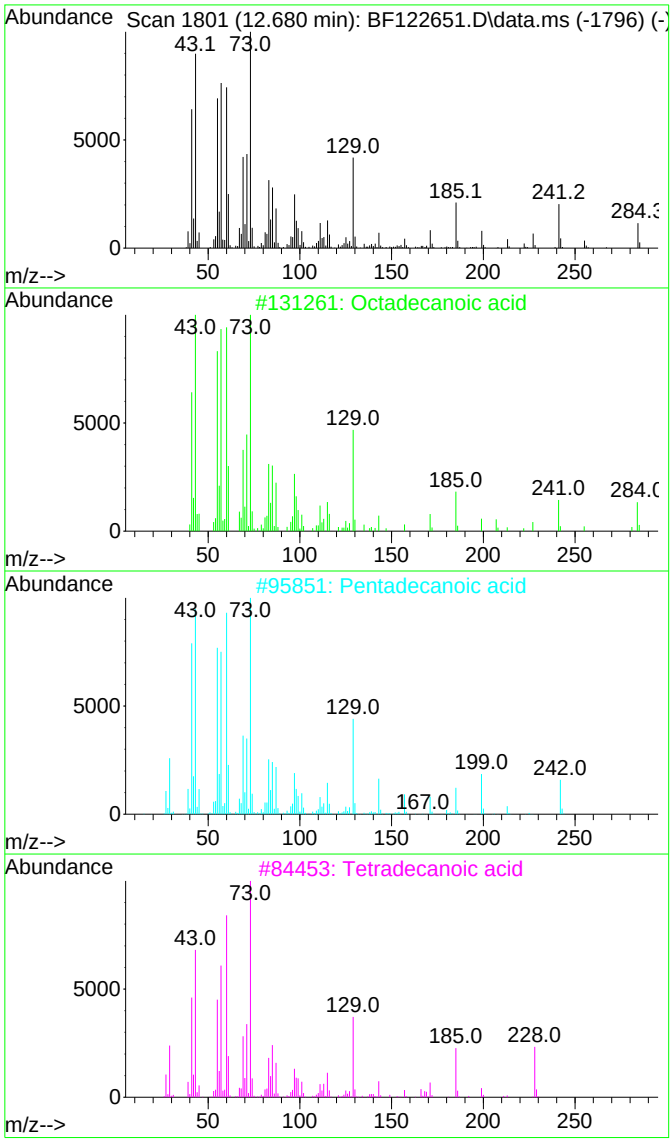
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

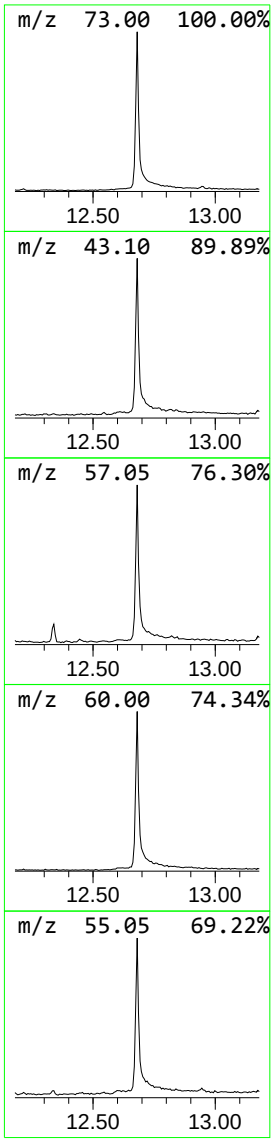
****

Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	12.53 ng	1196500	Phenanthrene-d10	11.363

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	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	70
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121020\
Data File : BF122651.D
Acq On : 10 Dec 2020 17:44
Operator : JU/CG
Sample : L4989-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-120920

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

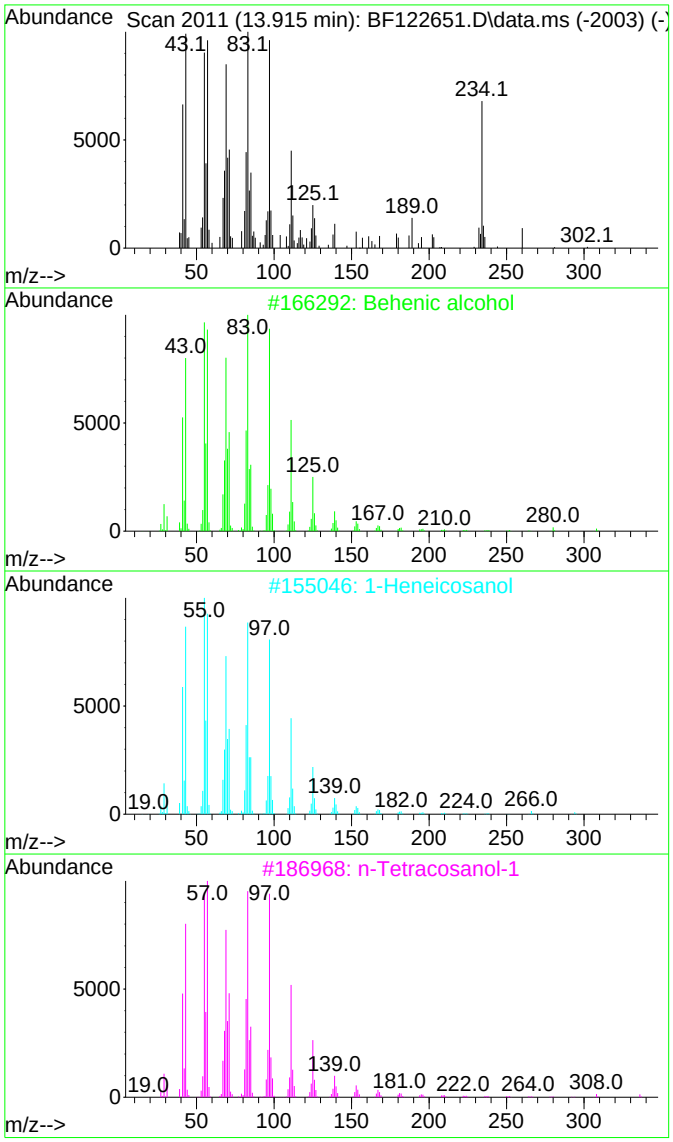
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

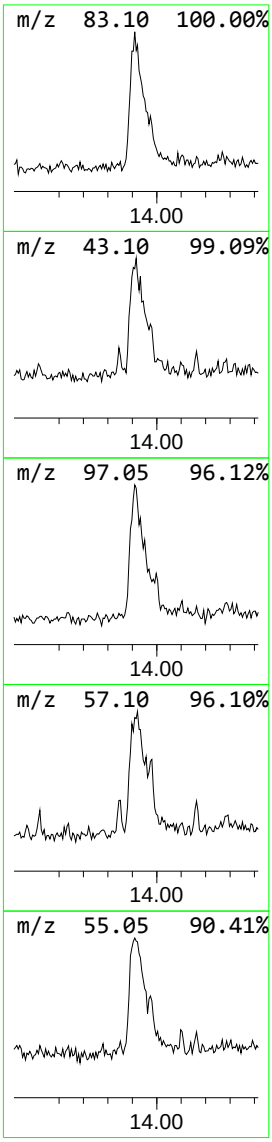
****

Peak Number 4 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	3.17 ng	310934	Chrysene-d12	13.998

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5	1-Nonadecene	266	C19H38	018435-45-5	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121020\
Data File : BF122651.D
Acq On : 10 Dec 2020 17:44
Operator : JU/CG
Sample : L4989-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-120920

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120520.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-...	5.057	2.3	ng	131170	1	6.839	1139100	20.0
n-Hexadecanoic ...	11.892	4.9	ng	467500	4	11.363	1909210	20.0
Octadecanoic acid	12.680	12.5	ng	1196500	4	11.363	1909210	20.0
Behenic alcohol	13.916	3.2	ng	310934	5	13.998	1959080	20.0