LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022221\
Data File : BF123269.D
Acq On : 22 Feb 2021 20:53
Operator : JU/CG
Sample : M1452-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-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-BF021921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123269.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	13	rVB	421223	497797	14.64%	1.748%
2	5.481	572	577	580	rBV	3331436	2999781	88.24%	10.534%
3	6.492	743	749	753	rBV2	3027601	3399706	100.00%	11.939%
4	6.857	807	811	814	rBV	926775	742646	21.84%	2.608%
5	7.416	901	906	909	rBV	2113259	2024899	59.56%	7.111%
6	8.139	1025	1029	1032	rBV	1218636	970212	28.54%	3.407%
7	9.216	1207	1212	1215	rBV	3692535	3226635	94.91%	11.331%
8	9.610	1276	1279	1283	rBV	83980	72365	2.13%	0.254%
9	9.757	1301	1304	1308	rVB	64497	47265	1.39%	0.166%
10	9.898	1324	1328	1331	rBV	1330157	1100954	32.38%	3.866%
11	10.686	1458	1462	1473	rBV	2225346	2185295	64.28%	7.674%
12	11.386	1577	1581	1584	rBV	1357036	1169009	34.39%	4.105%
13	11.410	1584	1585	1588	rVV	167262	98324	2.89%	0.345%
14	11.463	1591	1594	1597	rVB	44023	42783	1.26%	0.150%
15	11.922	1669	1672	1683	rBV	433284	515602	15.17%	1.811%
16	12.004	1683	1686	1688	rBV2	45939	43677	1.28%	0.153%
17	12.369	1746	1748	1751	rBV	56222	40781	1.20%	0.143%
18	12.439	1757	1760	1763	rBV	38455	39096	1.15%	0.137%
19	12.527	1772	1775	1780	rBV4	32684	35433	1.04%	0.124%
20	12.604	1784	1788	1793	rBV	454670	385296	11.33%	1.353%
21	12.710	1801	1806	1812	rBV3	90049	169133	4.97%	0.594%
22	12.833	1821	1827	1830	rBV	411097	380195	11.18%	1.335%
23	12.980	1848	1852	1855	rBV	3562447	3135233	92.22%	11.010%
24	13.051	1860	1864	1868	rBV4	41250	63151	1.86%	0.222%
25	13.139	1876	1879	1881	rBV3	42688	51563	1.52%	0.181%
26	13.163	1881	1883	1886	rVB	83313	63745	1.88%	0.224%
27	13.216	1888	1892	1893	rBV3	34434	39312	1.16%	0.138%
28	13.268	1897	1901	1904	rVV2	65741	65584	1.93%	0.230%
29	13.363	1914	1917	1919	rVB	40913	36602	1.08%	0.129%
30	13.392	1919	1922	1926	rBV	35921	40637	1.20%	0.143%
31	13.463	1932	1934	1940	rVB6	32030	36088	1.06%	0.127%
32	13.557	1947	1950	1958	rVB4	33901	45912	1.35%	0.161%
33	13.674	1967	1970	1974	rVB	53852	62492	1.84%	0.219%
34	13.786	1984	1989	1992	rBV2	45323	75456	2.22%	0.265%
35	13.910	2002	2010	2024	rBV4	190637	733930	21.59%	2.577%
36	14.039	2027	2032	2034	rVV2	1183314	1306238	38.42%	4.587%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022221\
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Acq On : 22 Feb 2021 20:53
Operator : JU/CG
Sample : M1452-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-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-BF021921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.063	2034	2036	2038	rVB	223302	163987	4.82%	0.576%
38	14.427	2095	2098	2101	rVB	48328	43999	1.29%	0.155%
39	14.510	2109	2112	2116	rVB3	68178	69782	2.05%	0.245%
40	14.551	2116	2119	2120	rBV3	44500	42377	1.25%	0.149%
41	15.080	2205	2209	2218	rVV	200603	383490	11.28%	1.347%
42	15.157	2220	2222	2225	rVV2	62060	58108	1.71%	0.204%
43	15.186	2225	2227	2231	rVB	47993	47691	1.40%	0.167%
44	15.380	2257	2260	2267	rVB	113899	159353	4.69%	0.560%
45	15.445	2267	2271	2277	rBV	164452	211542	6.22%	0.743%
46	15.510	2277	2282	2286	rBV	675333	843263	24.80%	2.961%
47	15.986	2360	2363	2368	rVB2	31163	41368	1.22%	0.145%
48	16.227	2400	2404	2415	rVB2	39966	94323	2.77%	0.331%
49	16.533	2453	2456	2461	rVB	24745	41610	1.22%	0.146%
50	16.662	2473	2478	2483	rVB8	20321	46440	1.37%	0.163%
51	16.980	2527	2532	2542	rVB2	76801	151922	4.47%	0.533%
52	17.427	2603	2608	2617	rVB	66020	134450	3.95%	0.472%

Sum of corrected areas: 28476532

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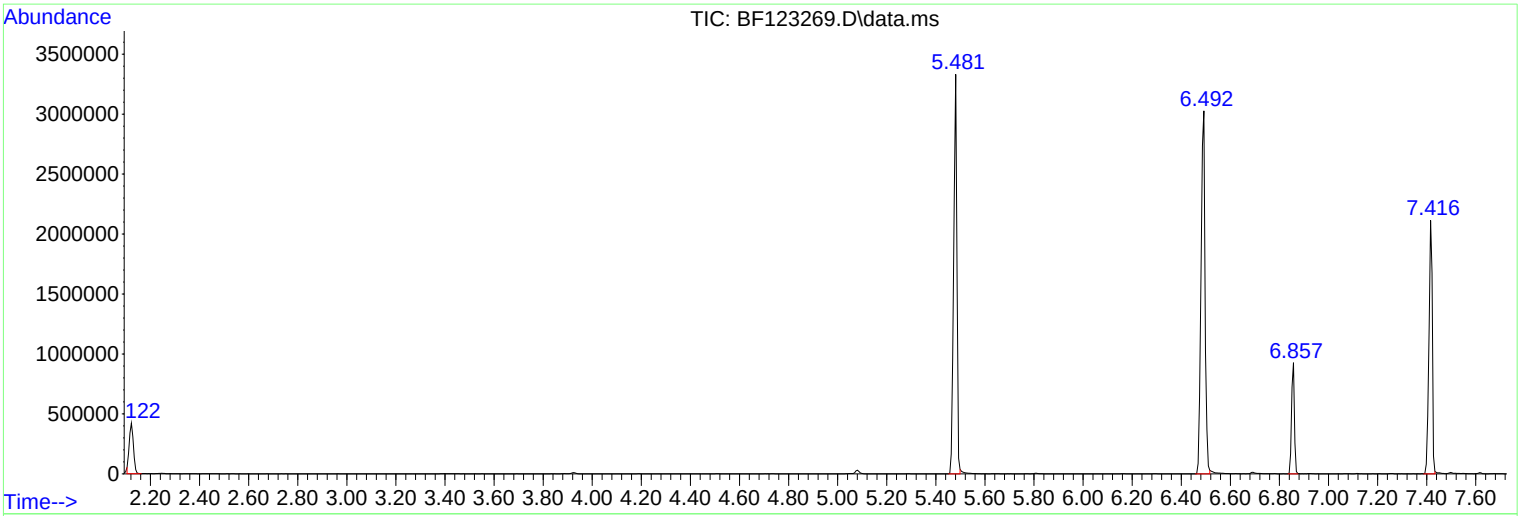
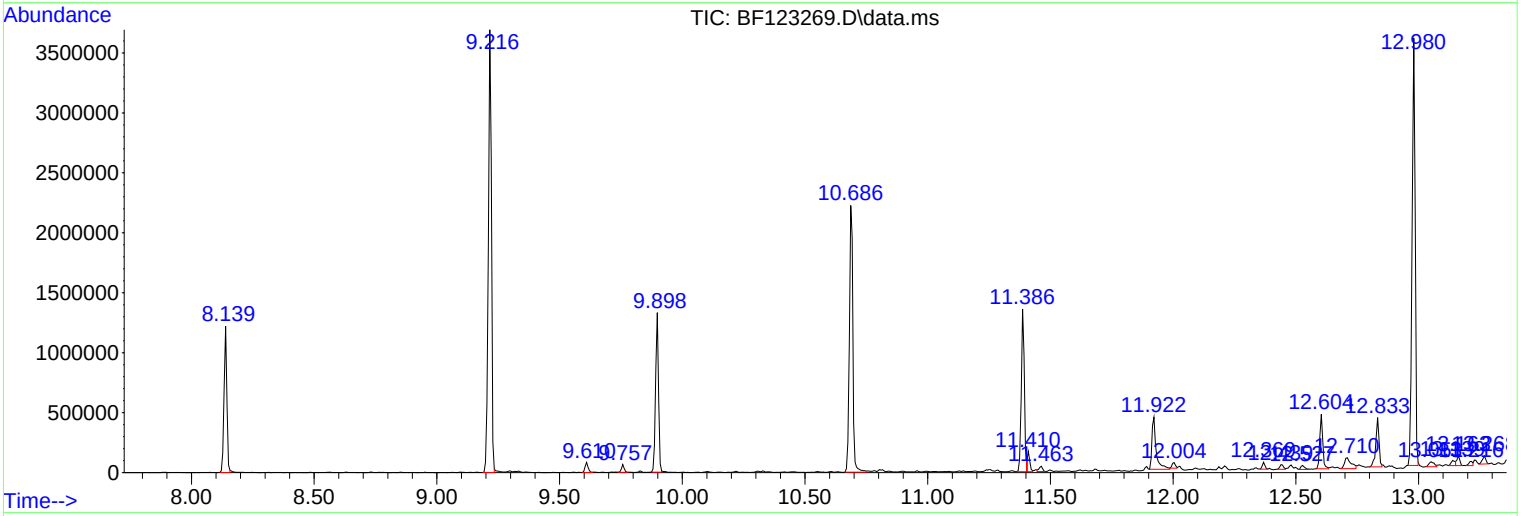
Misc :
ALS Vial : 18 Sample Multiplier: 1

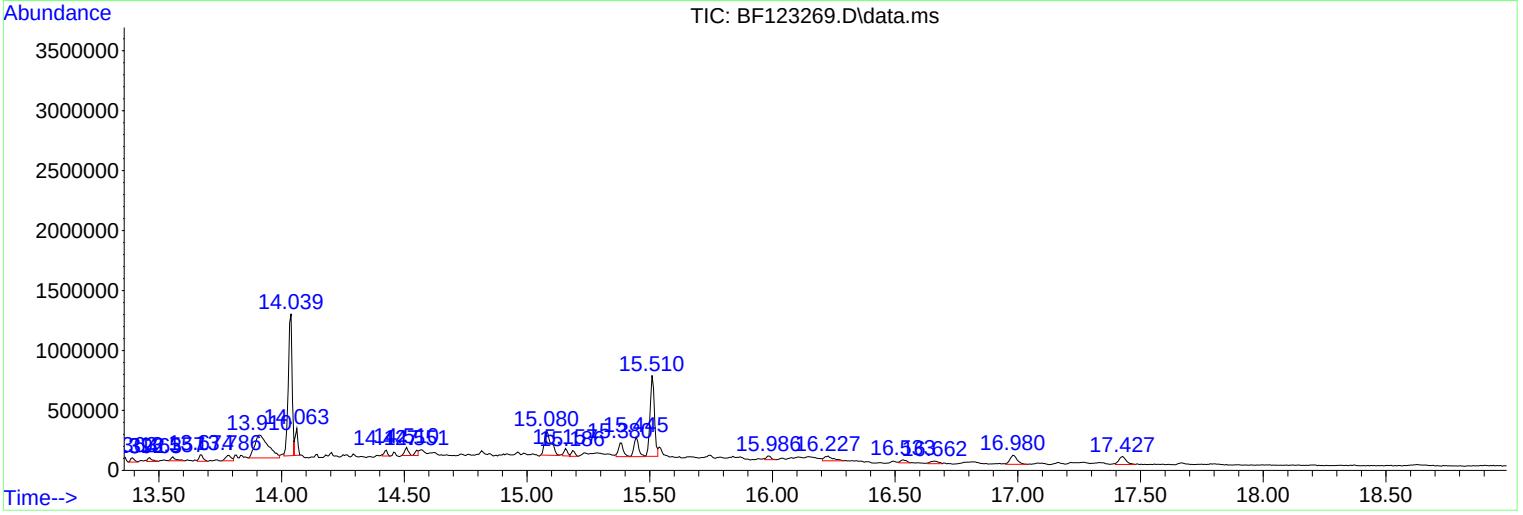
Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.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\BF022221\
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Operator : JU/CG
Sample : M1452-09
Misc :
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Instrument : BNA_F
ClientSampleId : TP-3

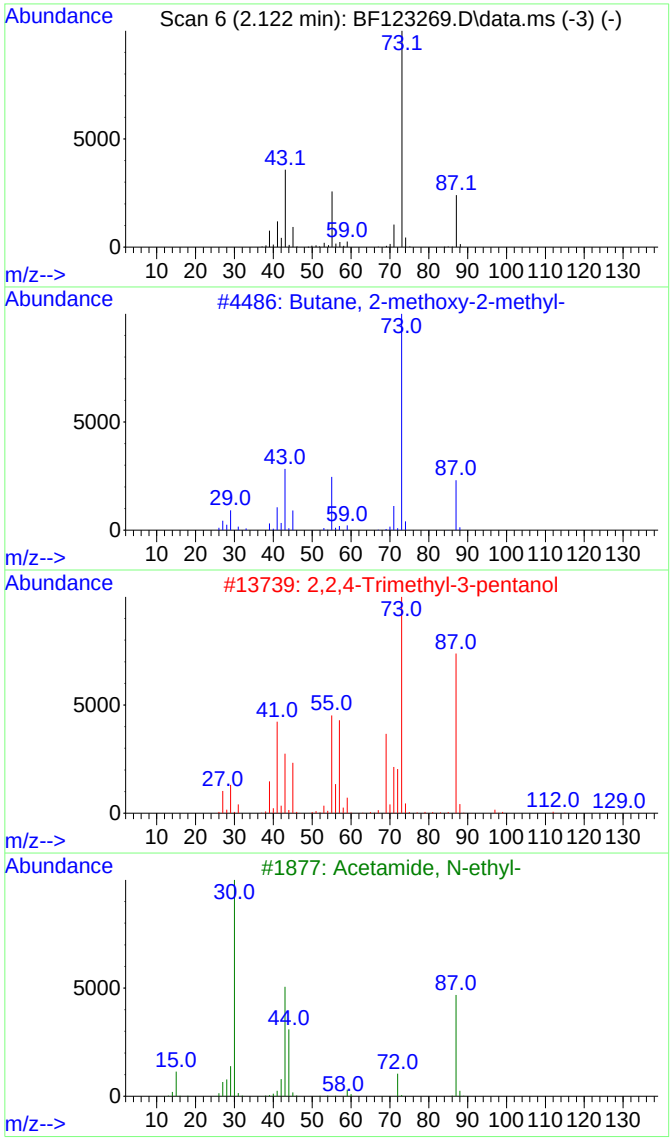
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

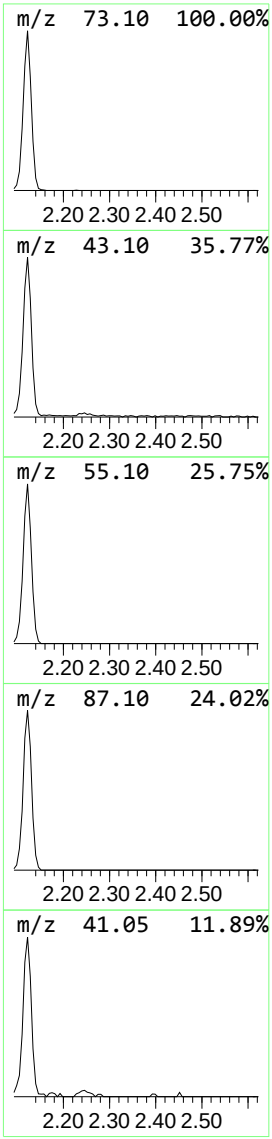
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	13.41 ng	497797	1,4-Dichlorobenzene-d4	6.857

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022221\
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Operator : JU/CG
Sample : M1452-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

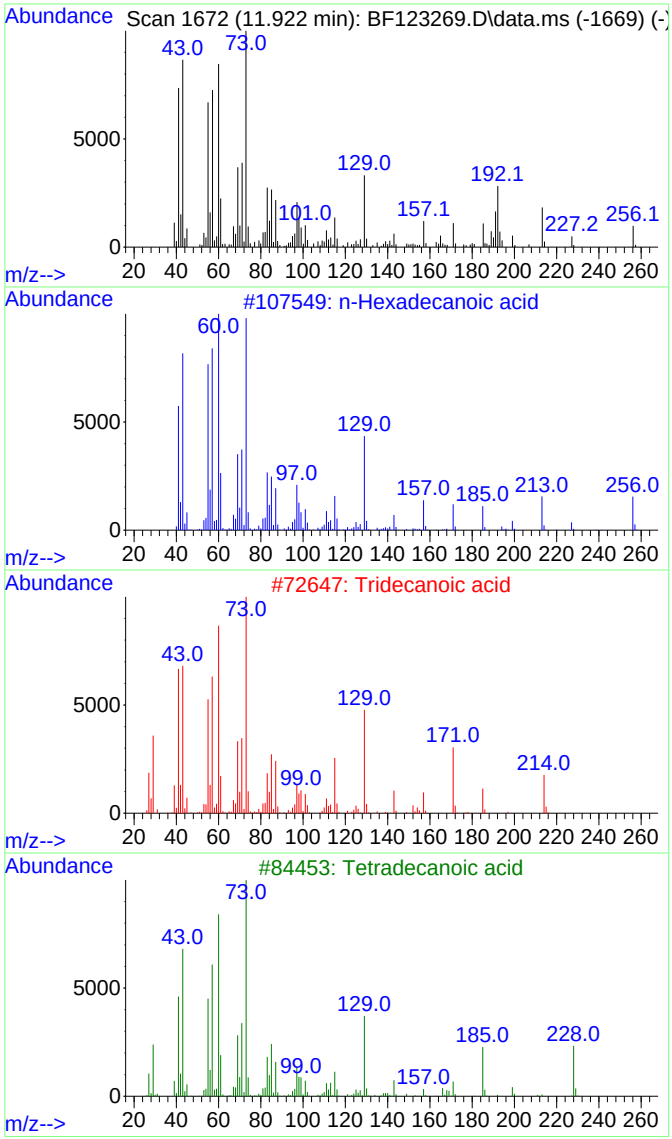
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

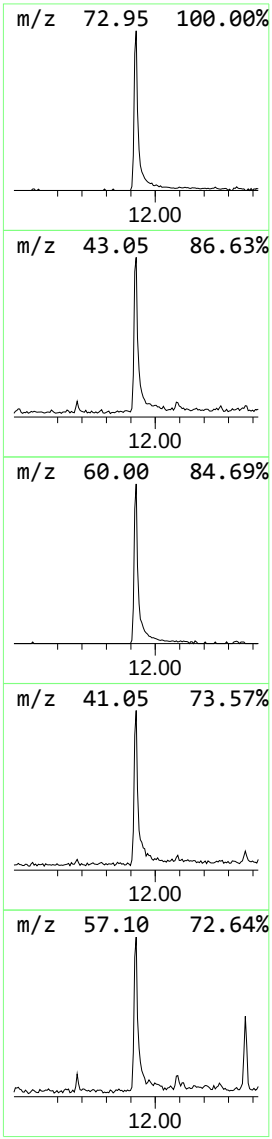
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	8.82 ng	515602	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022221\
Data File : BF123269.D
Acq On : 22 Feb 2021 20:53
Operator : JU/CG
Sample : M1452-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

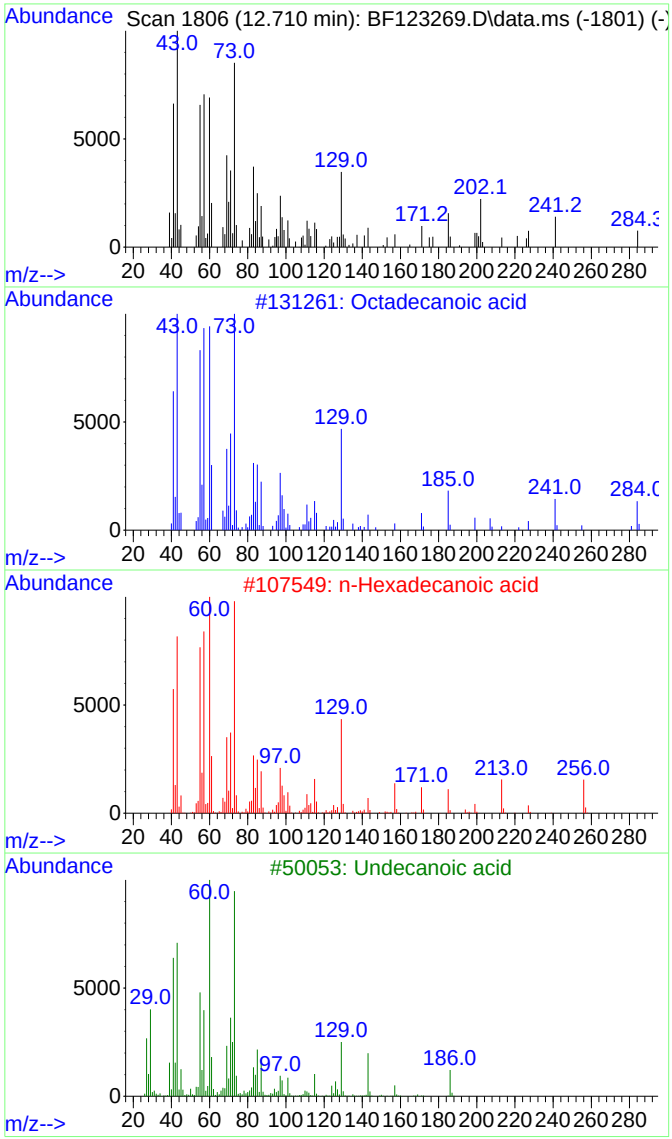
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

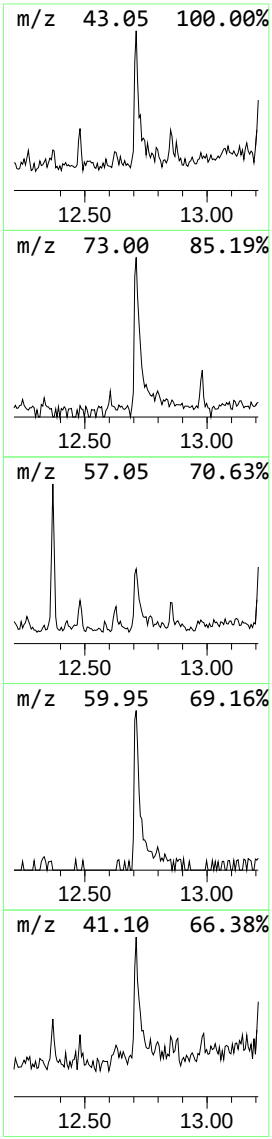
****

Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.710	2.89 ng	169133	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
3	Undecanoic acid	186	C11H22O2	000112-37-8	70
4	Dodecanoic acid	200	C12H24O2	000143-07-7	70
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	52





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Data File : BF123269.D
Acq On : 22 Feb 2021 20:53
Operator : JU/CG
Sample : M1452-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

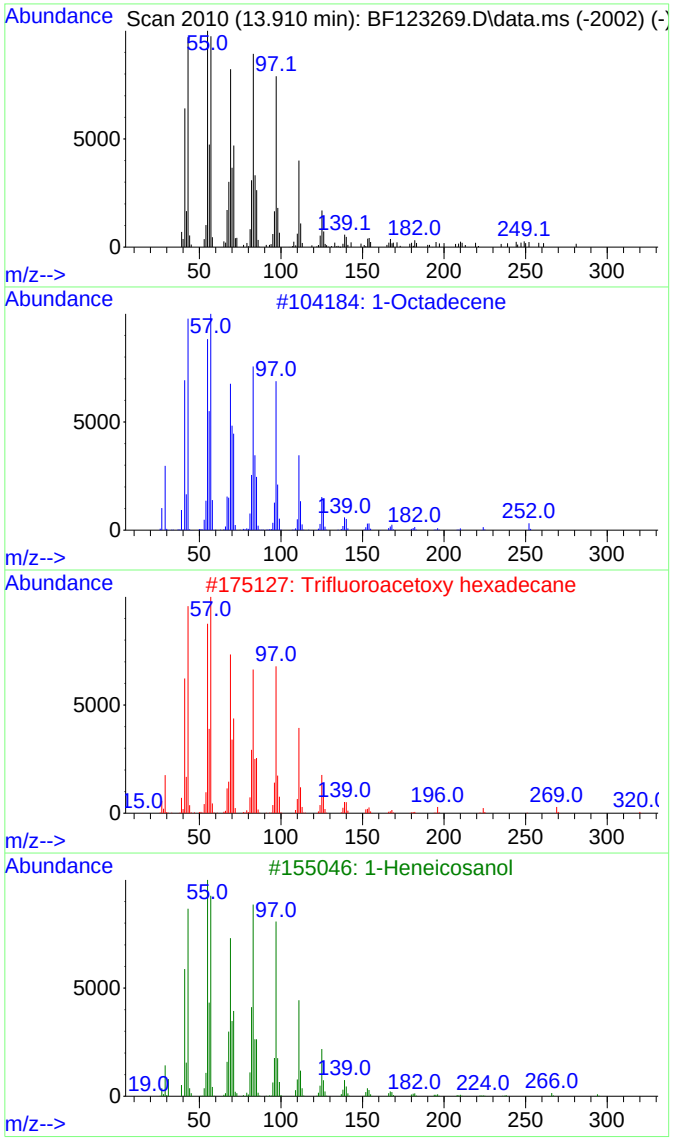
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

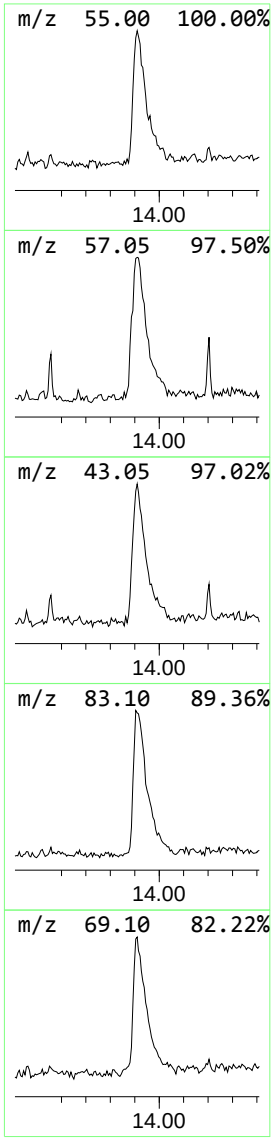
****

Peak Number 4 1-Octadecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	11.24 ng	733930	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	97
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94





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Sample : M1452-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

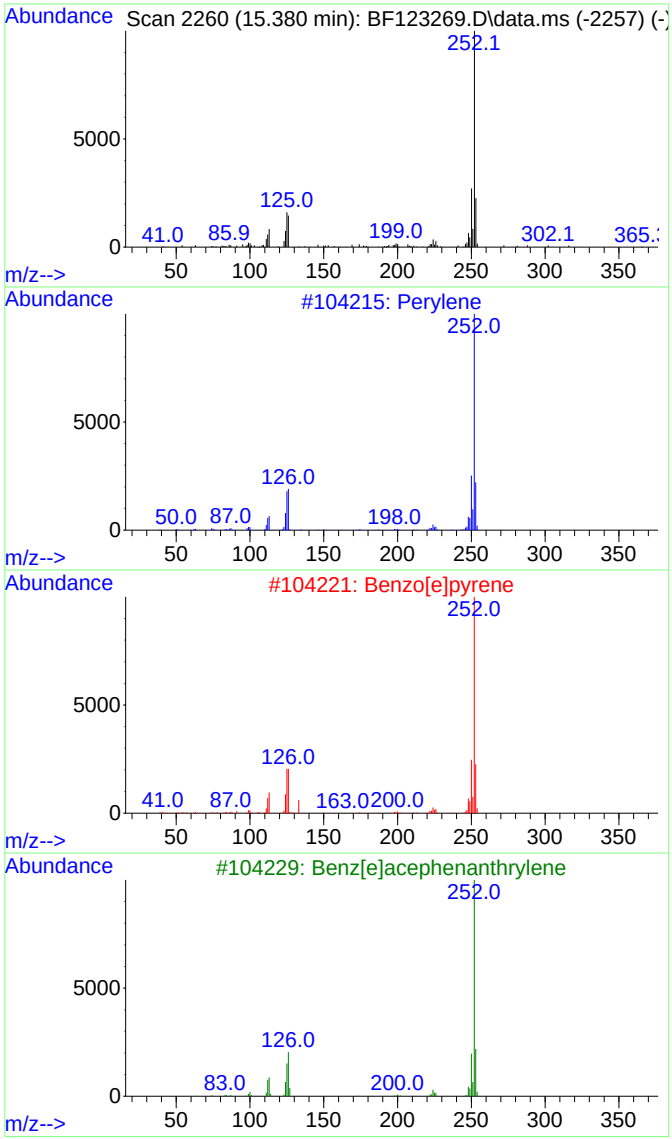
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

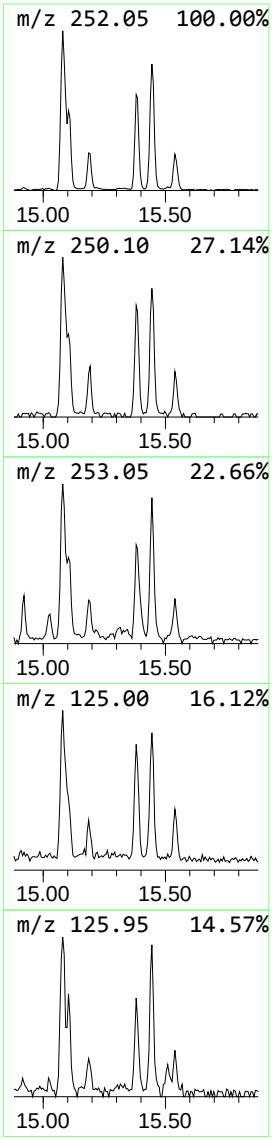
****

Peak Number 5 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.380	3.78 ng	159353	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	98
2	Benzo[e]pyrene	252	C20H12	000192-97-2	98
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	91





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Sample : M1452-09
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.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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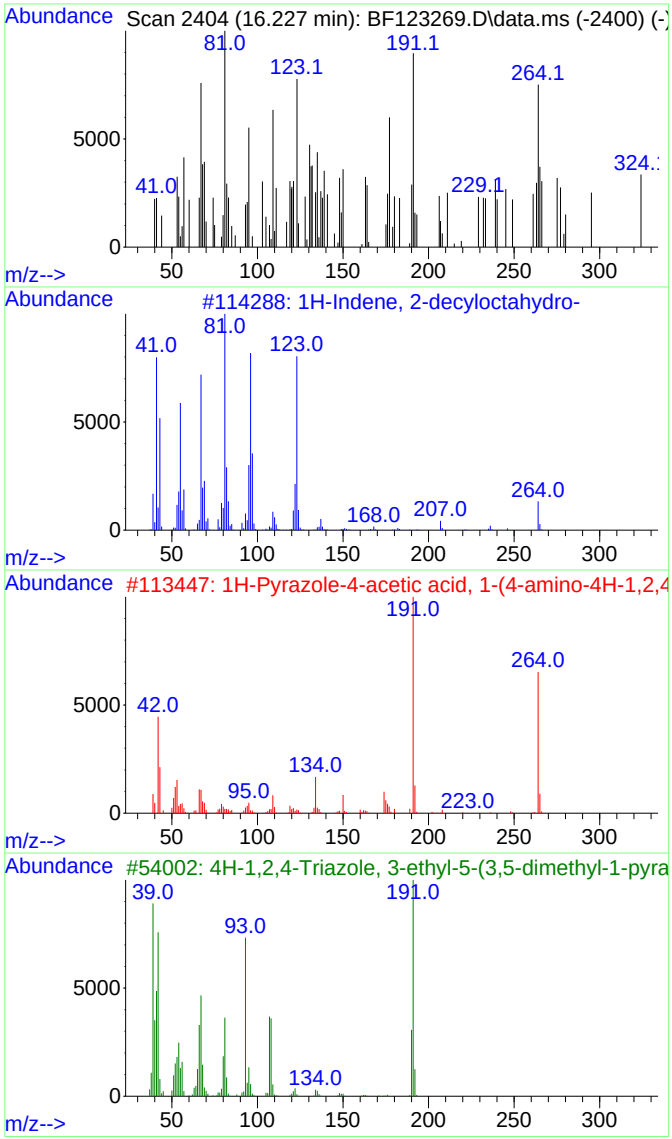
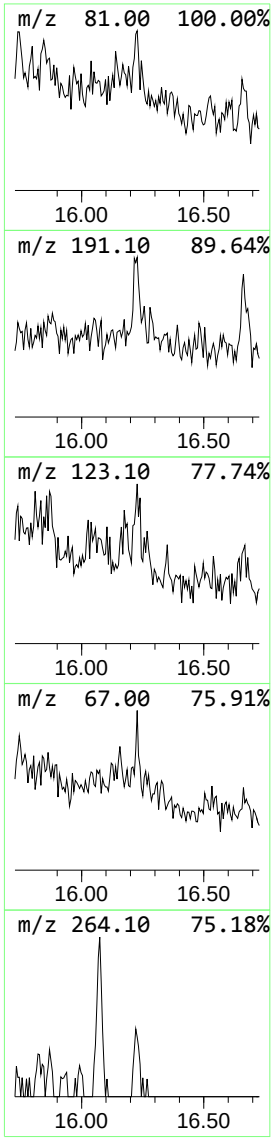
Peak Number 6 unknown16.227 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.227	2.24 ng	94323	Perylene-d12	15.509

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2-decyloctahydro-	264	C19H36	055044-34-3	38
2	1H-Pyrazole-4-acetic acid, 1-(4-...	264	C11H16N6O2	1000337-51-2	27
3	4H-1,2,4-Triazole, 3-ethyl-5-(3,...	191	C9H13N5	328532-29-2	25
4	Pyrimido(5,4-e)-as-triazine-5,7(...	179	C6H5N5O2	005016-18-2	22
5	[1,3,5]Triazine-2,4-diamine, 6-c...	295	C12H14ClN5O2	1000304-90-5	14





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.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-metho...	2.122	13.4	ng	497797	1	6.857	742646	20.0
n-Hexadecanoic ...	11.922	8.8	ng	515602	4	11.386	1169010	20.0
Octadecanoic acid	12.710	2.9	ng	169133	4	11.386	1169010	20.0
1-Octadecene	13.910	11.2	ng	733930	5	14.039	1306240	20.0
Perylene	15.380	3.8	ng	159353	6	15.509	843263	20.0
unknown16.227	16.227	2.2	ng	94323	6	15.509	843263	20.0