LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030121\
Data File : BF123329.D
Acq On : 1 Mar 2021 16:35
Operator : JU/CG
Sample : M1499-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

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

Signal : TIC: BF123329.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	3	9	19	rVB4	52422	129615	2.06%	0.227%
2	2.357	36	46	59	rVB	870321	1111656	17.63%	1.946%
3	5.140	515	519	529	rVB	63504	96726	1.53%	0.169%
4	5.504	576	581	584	rBV	5126728	5636984	89.42%	9.870%
5	6.492	743	749	766	rVB	4349353	5972341	94.73%	10.457%
6	6.851	806	810	814	rBV	1963665	1628611	25.83%	2.852%
7	7.416	899	906	909	rBV	3185672	3870776	61.40%	6.778%
8	8.134	1022	1028	1032	rBV	2162585	2154103	34.17%	3.772%
9	9.216	1204	1212	1215	rBV	5813874	6304272	100.00%	11.039%
10	9.604	1270	1278	1282	rBV2	341815	366498	5.81%	0.642%
11	9.751	1300	1303	1307	rVB	290120	236860	3.76%	0.415%
12	9.892	1320	1327	1331	rBV	2441030	2313426	36.70%	4.051%
13	10.210	1377	1381	1384	rBV3	50643	68760	1.09%	0.120%
14	10.686	1455	1462	1465	rBV	3692526	3693551	58.59%	6.467%
15	10.810	1479	1483	1486	rVB3	94439	130770	2.07%	0.229%
16	11.245	1553	1557	1561	rBV5	61676	90194	1.43%	0.158%
17	11.280	1561	1563	1567	rVB	64985	63756	1.01%	0.112%
18	11.386	1574	1581	1583	rBV	2300801	2096533	33.26%	3.671%
19	11.404	1583	1584	1587	rVV	286008	224655	3.56%	0.393%
20	11.457	1591	1593	1596	rVB	128478	104665	1.66%	0.183%
21	11.774	1642	1647	1650	rBV	1013747	874134	13.87%	1.531%
22	11.845	1656	1659	1663	rBV	51228	64174	1.02%	0.112%
23	11.886	1663	1666	1668	rBV	122400	123309	1.96%	0.216%
24	11.916	1668	1671	1677	rVB	1069116	961975	15.26%	1.684%
25	11.998	1682	1685	1687	rBV2	102216	115546	1.83%	0.202%
26	12.210	1718	1721	1724	rVB2	137695	144162	2.29%	0.252%
27	12.363	1744	1747	1750	rVB	455422	370424	5.88%	0.649%
28	12.421	1754	1757	1758	rBV	87611	81074	1.29%	0.142%
29	12.439	1758	1760	1761	rVV	90494	82227	1.30%	0.144%
30	12.469	1761	1765	1767	rVV	3184673	3001739	47.61%	5.256%
31	12.486	1767	1768	1773	rVB2	2320827	1825964	28.96%	3.197%
32	12.574	1780	1783	1785	rBV	392128	313187	4.97%	0.548%
33	12.604	1785	1788	1790	rBV	390781	374312	5.94%	0.655%
34	12.704	1801	1805	1808	rBV2	390534	412047	6.54%	0.721%
35	12.769	1813	1816	1819	rVB	136161	111241	1.76%	0.195%
36	12.827	1823	1826	1832	rVB	406037	435217	6.90%	0.762%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030121\
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Acq On : 1 Mar 2021 16:35
Operator : JU/CG
Sample : M1499-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

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

37	12.980	1844	1852	1855	rBV	5264703	5270286	83.60%	9.228%
38	13.051	1861	1864	1868	rBV3	67459	82170	1.30%	0.144%
39	13.263	1898	1900	1903	rVB2	84958	80000	1.27%	0.140%
40	13.333	1909	1912	1914	rBV3	64994	77475	1.23%	0.136%
41	13.668	1967	1969	1974	rVB	96485	91930	1.46%	0.161%
42	13.880	2002	2005	2016	rVB	618038	937314	14.87%	1.641%
43	14.039	2027	2032	2034	rBV	1817017	1870725	29.67%	3.276%
44	14.063	2034	2036	2040	rVB	268469	229665	3.64%	0.402%
45	14.504	2109	2111	2113	rBV2	92409	81234	1.29%	0.142%
46	15.080	2206	2209	2212	rBV	302224	405230	6.43%	0.710%
47	15.386	2258	2261	2267	rVB	251373	311291	4.94%	0.545%
48	15.451	2268	2272	2277	rVV	259334	362859	5.76%	0.635%
49	15.515	2278	2283	2294	rVB	1148627	1725392	27.37%	3.021%

Sum of corrected areas: 57111055

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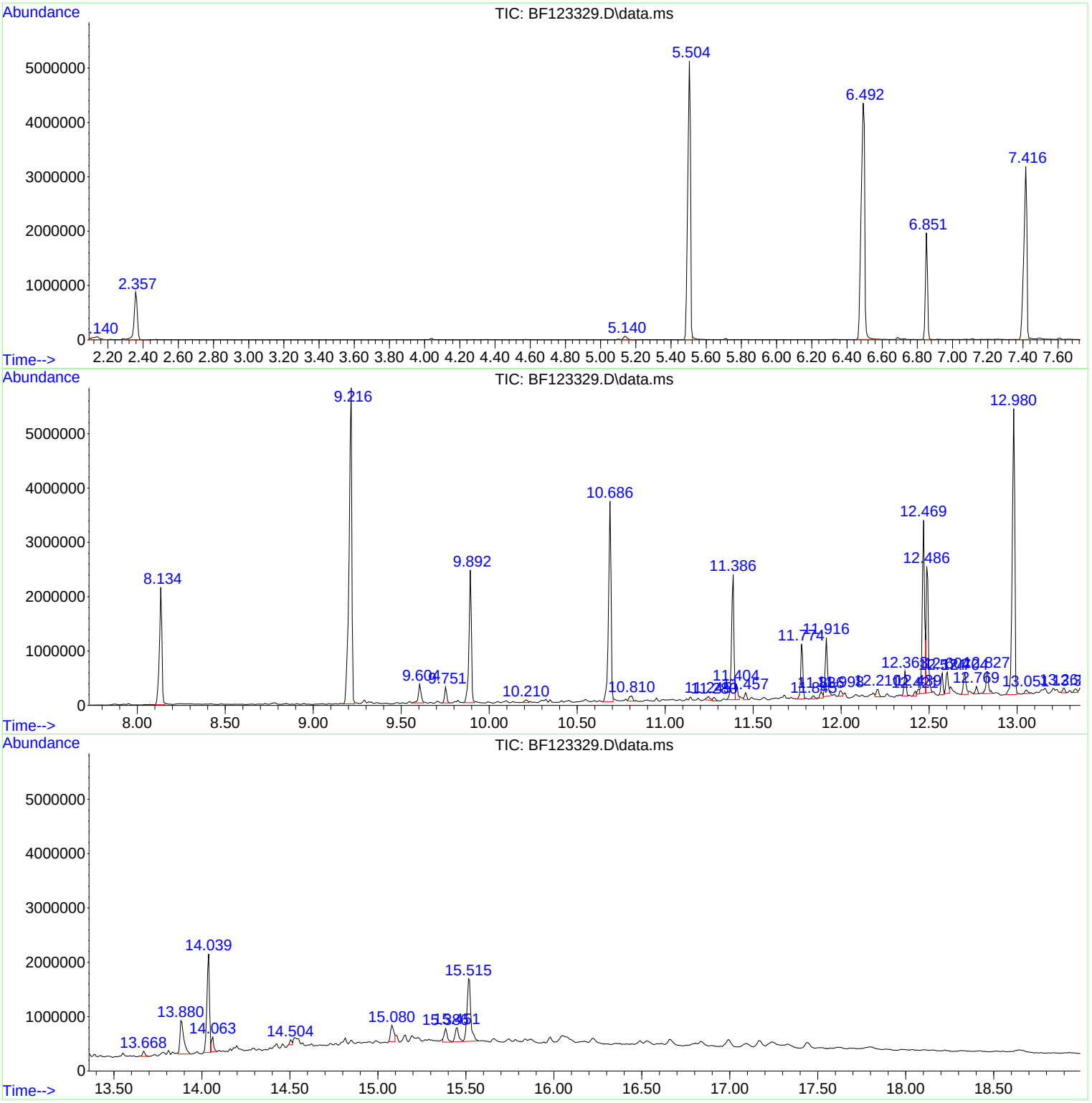
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N-1

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\BF030121\
Data File : BF123329.D
Acq On : 1 Mar 2021 16:35
Operator : JU/CG
Sample : M1499-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-1

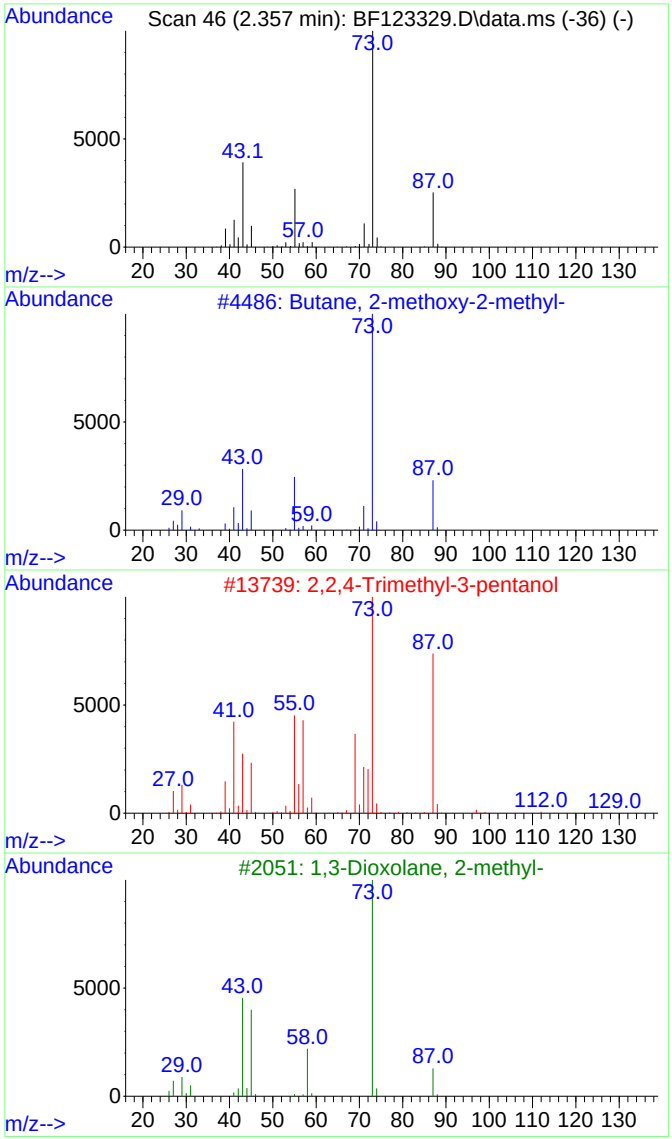
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

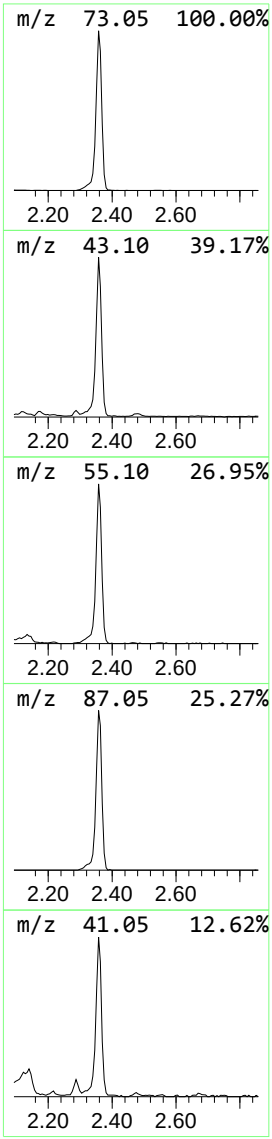
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.357	13.65 ng	1111660	1,4-Dichlorobenzene-d4	6.851

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9





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Data File : BF123329.D
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Operator : JU/CG
Sample : M1499-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-1

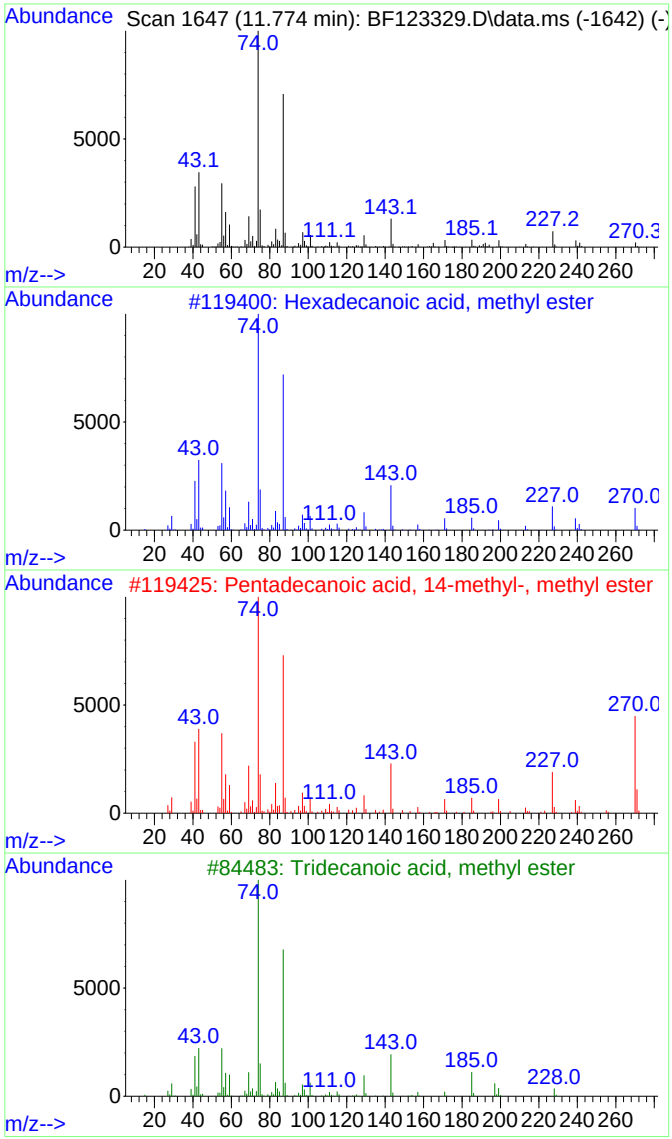
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

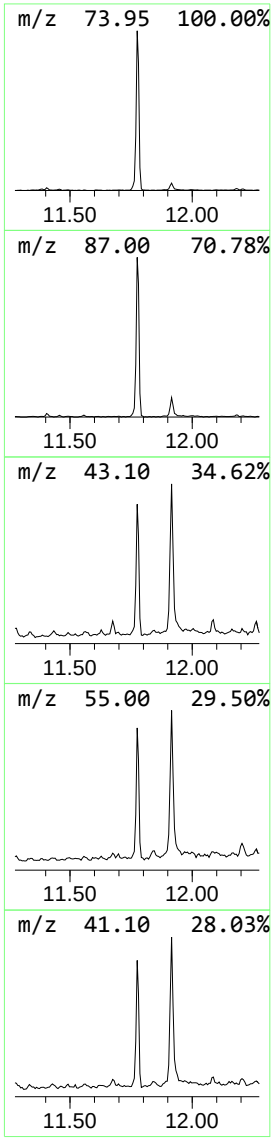
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.775	8.34 ng	874134	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	92
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87





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Operator : JU/CG
Sample : M1499-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-1

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

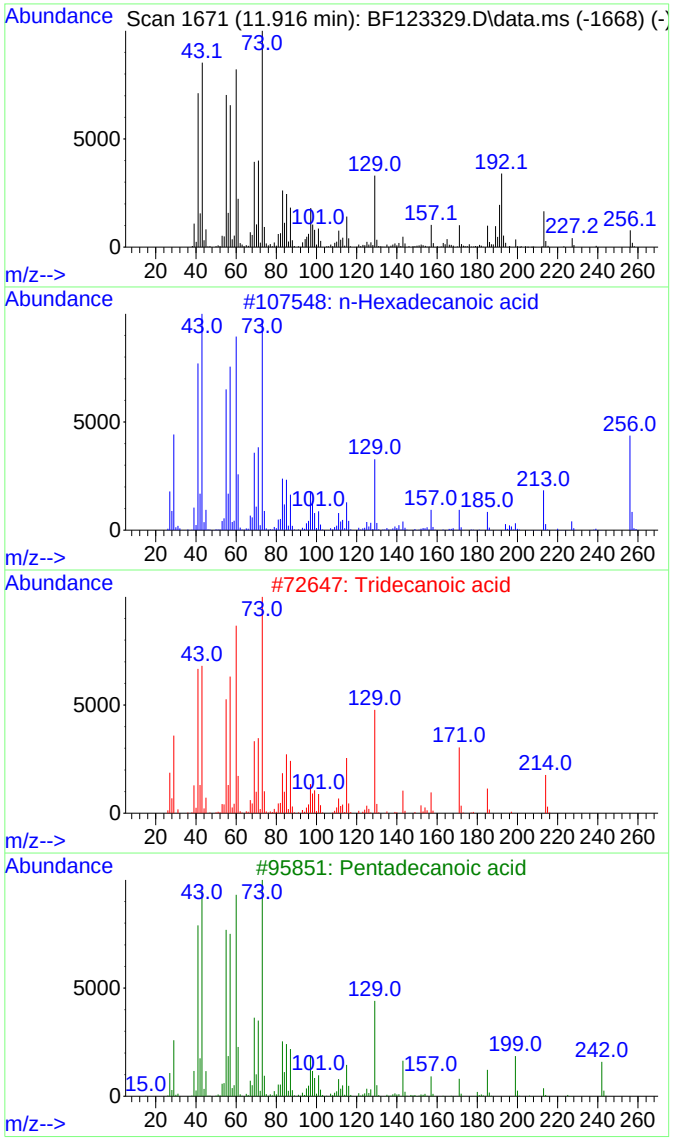
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

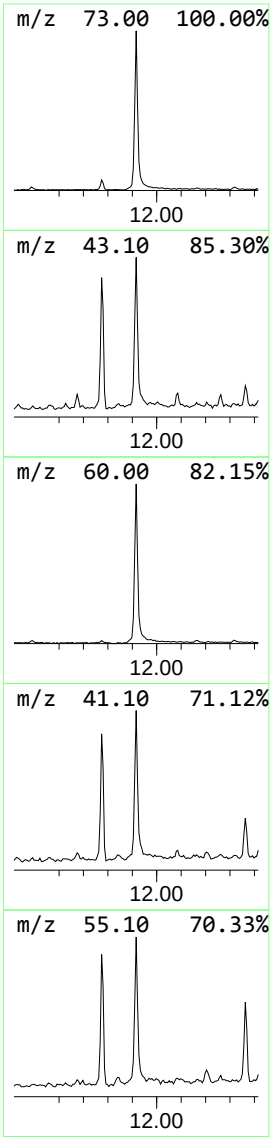
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	9.18 ng	961975	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	96
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Methyl isopropylidene-.beta.-d-a...	204	C9H16O5	1000129-88-1	53





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Operator : JU/CG
Sample : M1499-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-1

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

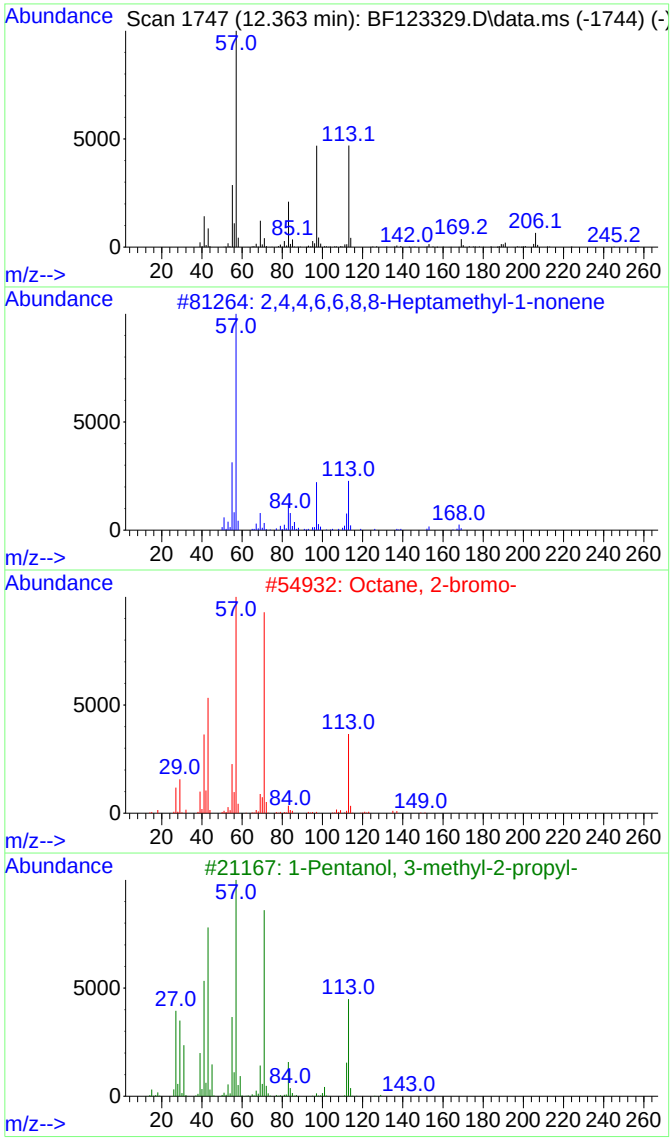
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

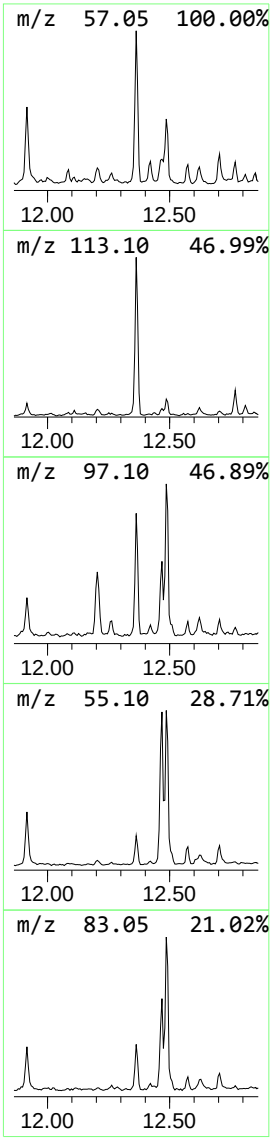
****

Peak Number 4 unknown12.36 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.363	3.53 ng	370424	Phenanthrene-d10	11.386

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	Octane, 2-bromo-	192	C8H17Br	000557-35-7	32
3	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	28
4	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	25
5	Cyclohexane, 1,1'-[1,2-bis(1,1-d...	306	C22H42	065149-85-1	25





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Sample : M1499-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N-1

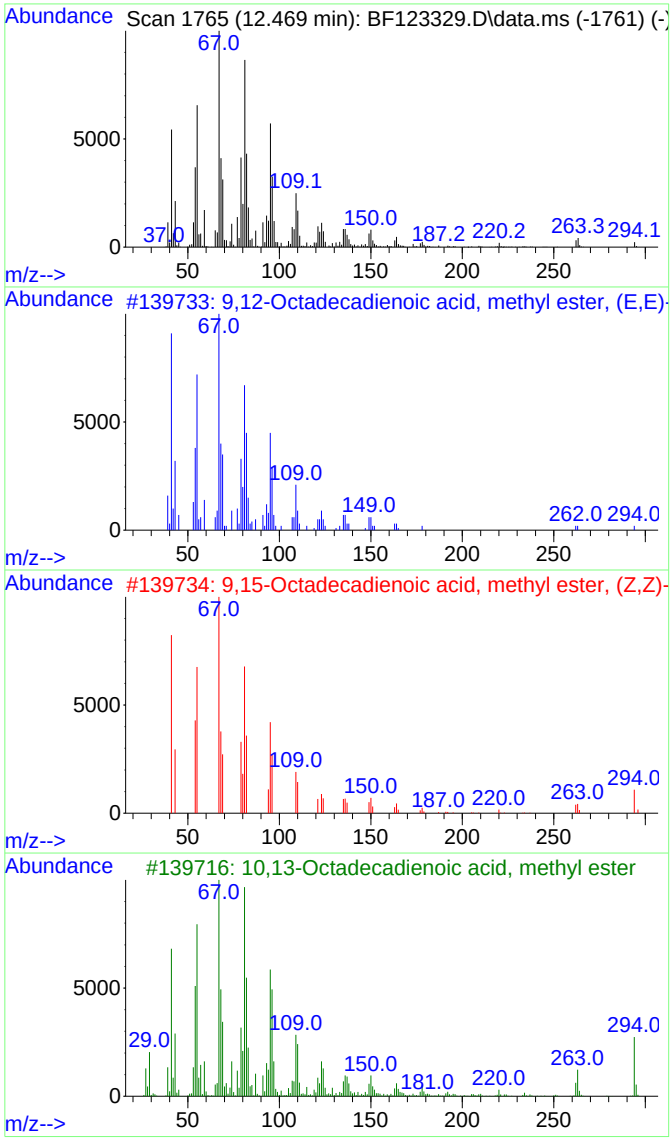
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

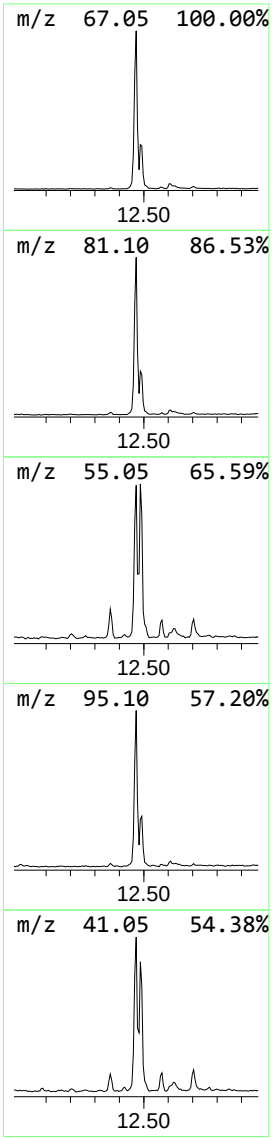
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	28.64 ng	3001740	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	98
4	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	98
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	98





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ALS Vial : 12 Sample Multiplier: 1

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BNA_F
ClientSampleId :
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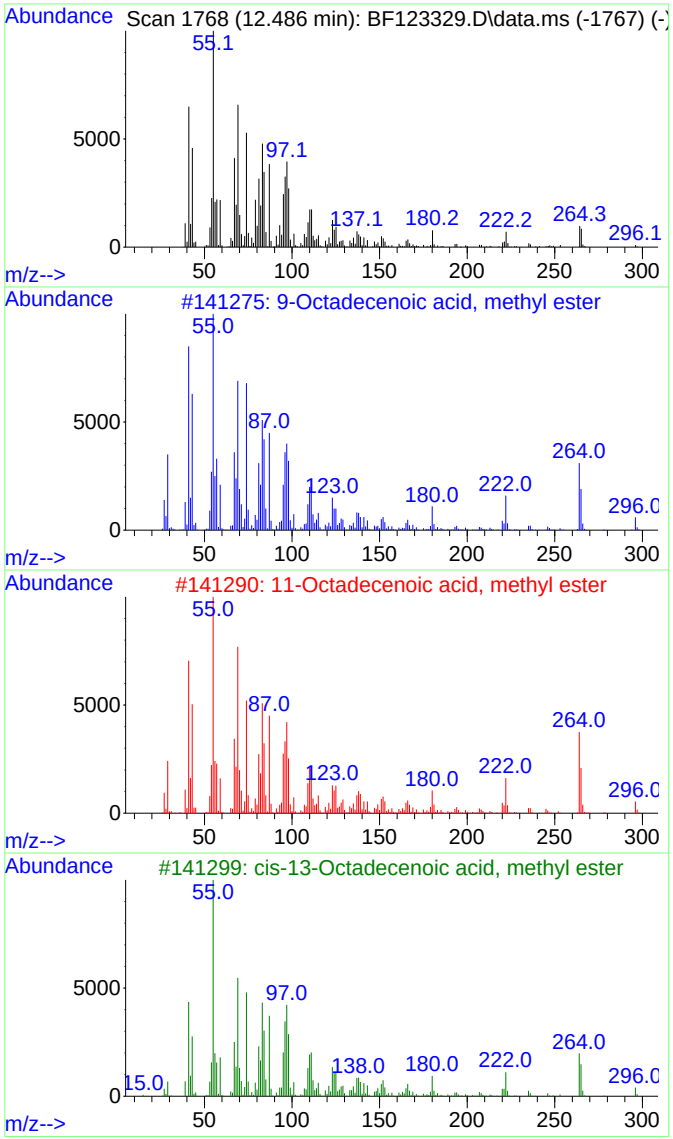
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

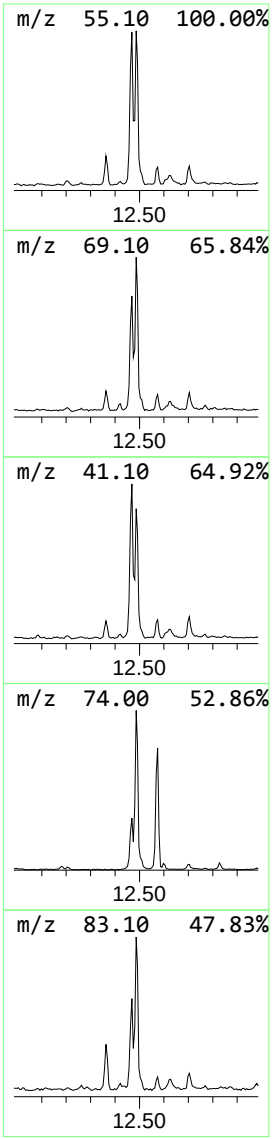
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 9-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.486	17.42 ng	1825960	Phenanthrene-d10	11.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
3	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	99
4	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	99
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99





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ALS Vial : 12 Sample Multiplier: 1

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

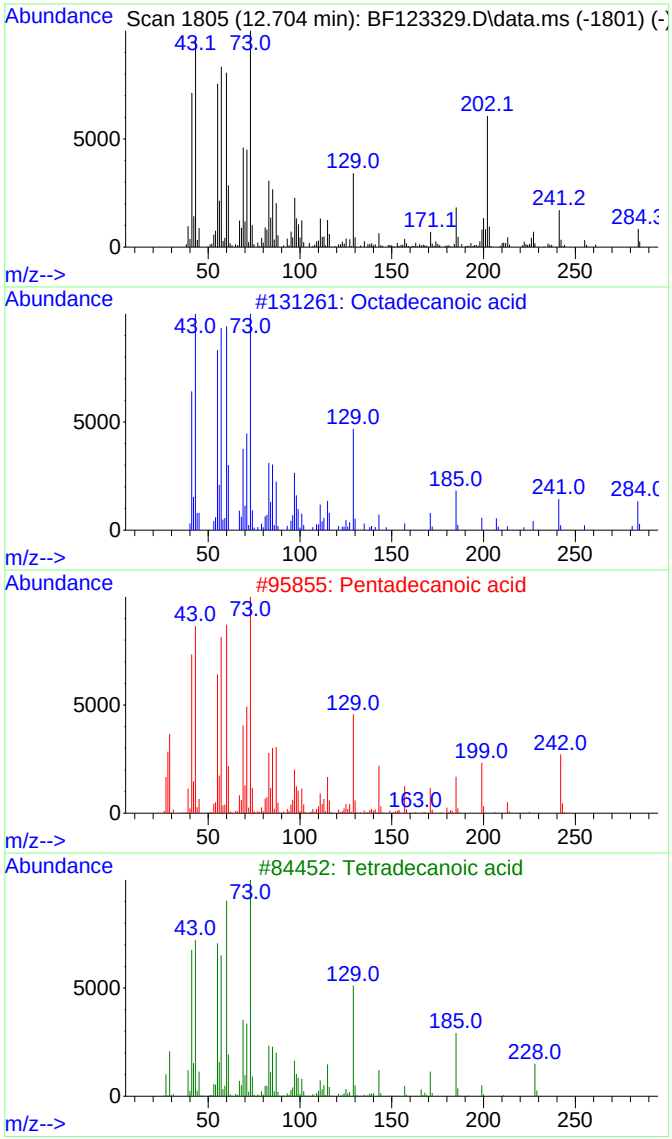
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

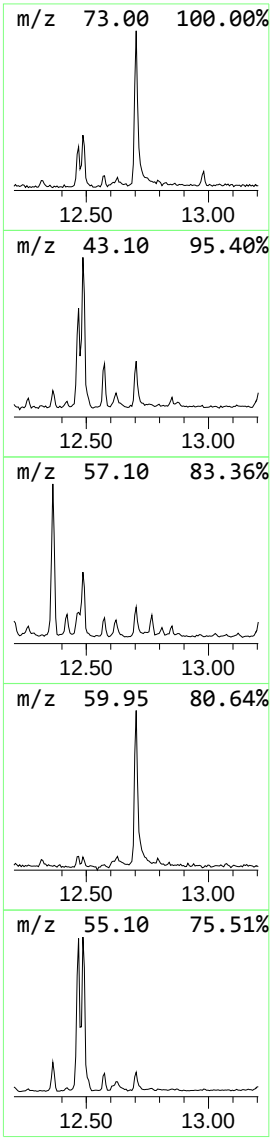
****

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	3.93 ng	412047	Phenanthrene-d10	11.386

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	86
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030121\
Data File : BF123329.D
Acq On : 1 Mar 2021 16:35
Operator : JU/CG
Sample : M1499-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-1

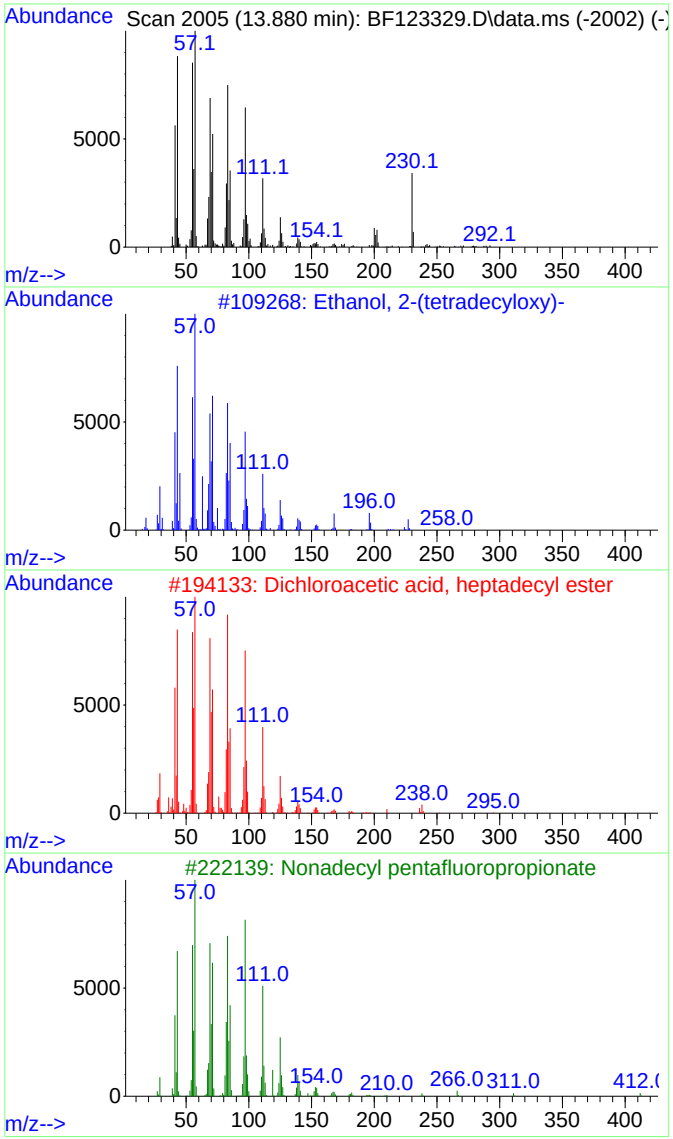
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

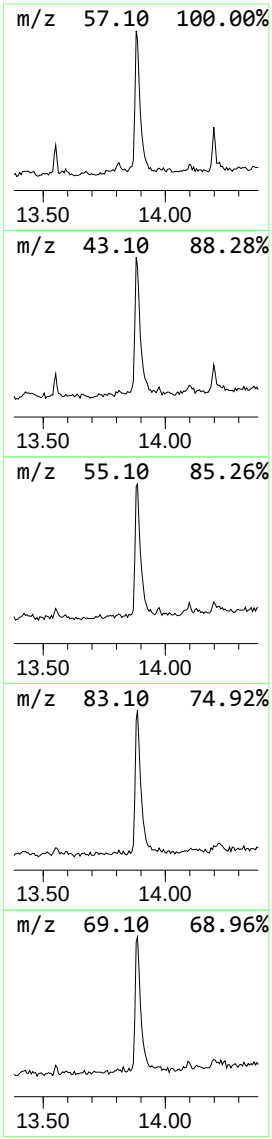
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	10.02 ng	937314	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	93
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
4	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030121\
Data File : BF123329.D
Acq On : 1 Mar 2021 16:35
Operator : JU/CG
Sample : M1499-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-1

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

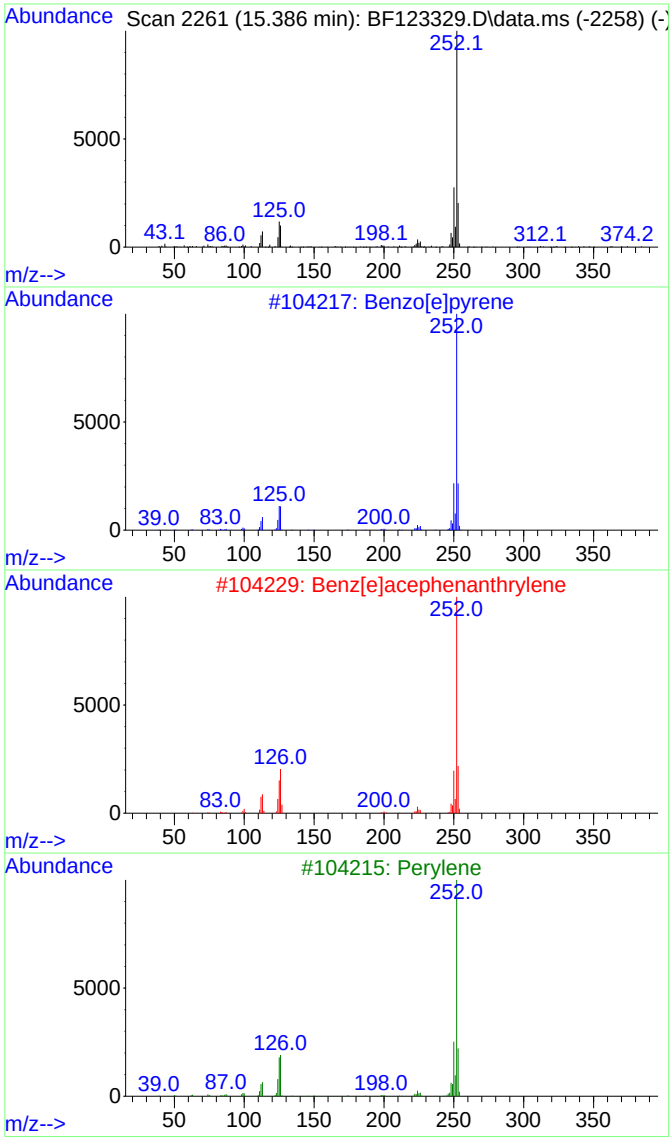
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

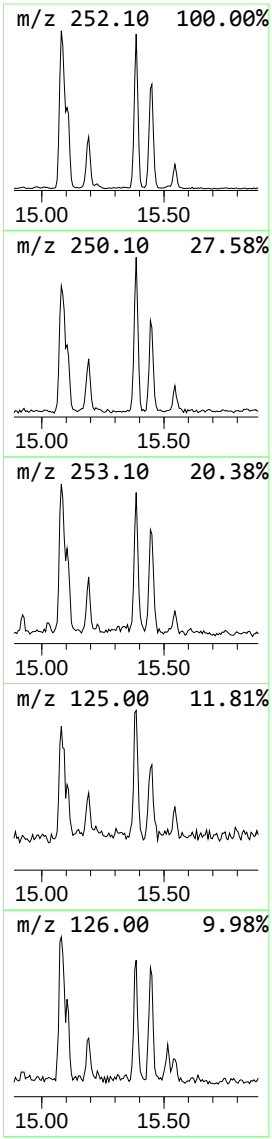
****

Peak Number 9 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.386	3.61 ng	311291	Perylene-d12	15.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
3	Perylene	252	C20H12	000198-55-0	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030121\
Data File : BF123329.D
Acq On : 1 Mar 2021 16:35
Operator : JU/CG
Sample : M1499-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-1

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...	2.357	13.7	ng	1111660	1	6.851	1628610	20.0
Hexadecanoic ac...	11.775	8.3	ng	874134	4	11.386	2096530	20.0
n-Hexadecanoic ...	11.916	9.2	ng	961975	4	11.386	2096530	20.0
unknown12.36	12.363	3.5	ng	370424	4	11.386	2096530	20.0
9,12-Octadecadi...	12.469	28.6	ng	3001740	4	11.386	2096530	20.0
9-Octadecenoic ...	12.486	17.4	ng	1825960	4	11.386	2096530	20.0
Octadecanoic acid	12.704	3.9	ng	412047	4	11.386	2096530	20.0
Ethanol, 2-(tet...	13.880	10.0	ng	937314	5	14.039	1870730	20.0
Benzo[e]pyrene	15.386	3.6	ng	311291	6	15.515	1725390	20.0