LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122194.D
Acq On : 30 Oct 2020 22:23
Operator : JU/CG
Sample : L4565-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-063-A

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-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122194.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.339	550	553	581	rBV	1871882	2437880	88.90%	10.735%
2	6.369	725	728	755	rBV	2241821	2597419	94.72%	11.438%
3	6.592	763	766	782	rBV	22602	75303	2.75%	0.332%
4	6.710	782	786	798	rVB	689432	681790	24.86%	3.002%
5	7.281	880	883	899	rBV	1605467	1613952	58.85%	7.107%
6	7.992	1001	1004	1019	rVB	949091	914662	33.35%	4.028%
7	8.439	1077	1080	1099	rBV2	42440	102690	3.74%	0.452%
8	9.069	1183	1187	1196	rBV	3116155	2742272	100.00%	12.076%
9	9.186	1203	1207	1212	rVB	76973	74399	2.71%	0.328%
10	9.469	1252	1255	1265	rVB	456784	415314	15.14%	1.829%
11	9.745	1298	1302	1306	rBV	1188200	1009259	36.80%	4.444%
12	9.780	1306	1308	1313	rVB	33244	31655	1.15%	0.139%
13	10.145	1367	1370	1372	rBV	36433	32464	1.18%	0.143%
14	10.539	1433	1437	1448	rBV	1741112	1688945	61.59%	7.437%
15	10.645	1452	1455	1464	rVB4	24106	44318	1.62%	0.195%
16	11.086	1525	1530	1533	rBV3	27966	36279	1.32%	0.160%
17	11.233	1551	1555	1558	rBV	1054181	951703	34.70%	4.191%
18	11.257	1558	1559	1566	rVV	254465	225990	8.24%	0.995%
19	11.321	1567	1570	1578	rVB	56964	72618	2.65%	0.320%
20	11.739	1639	1641	1643	rBV	39763	36200	1.32%	0.159%
21	11.763	1643	1645	1653	rVB3	114848	155839	5.68%	0.686%
22	11.851	1658	1660	1663	rBV	64355	57027	2.08%	0.251%
23	12.286	1731	1734	1736	rBV	38908	37353	1.36%	0.164%
24	12.451	1758	1762	1768	rBV	484365	458533	16.72%	2.019%
25	12.680	1795	1801	1804	rBV	423310	450722	16.44%	1.985%
26	12.815	1820	1824	1828	rBV	2436680	2100186	76.59%	9.248%
27	12.904	1835	1839	1845	rVB3	35634	64438	2.35%	0.284%
28	12.986	1850	1853	1856	rVV5	25119	39963	1.46%	0.176%
29	13.033	1860	1861	1864	rVB	40778	31400	1.15%	0.138%
30	13.080	1866	1869	1872	rVV2	39465	38021	1.39%	0.167%
31	13.121	1872	1876	1879	rVV2	40785	53474	1.95%	0.235%
32	13.210	1888	1891	1894	rBV	34061	36423	1.33%	0.160%
33	13.239	1894	1896	1901	rVV3	31623	42619	1.55%	0.188%
34	13.380	1917	1920	1923	rBV2	63916	67597	2.46%	0.298%
35	13.710	1973	1976	1982	rBV	204327	274400	10.01%	1.208%
36	13.880	2000	2005	2008	rBV2	713563	841021	30.67%	3.703%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122194.D
Acq On : 30 Oct 2020 22:23
Operator : JU/CG
Sample : L4565-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-063-A

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-BF101220.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.909	2008	2010	2017	rVB	192753	202306	7.38%	0.891%
38	14.021	2027	2029	2032	rBV	49431	47163	1.72%	0.208%
39	14.621	2129	2131	2134	rVB2	53232	47211	1.72%	0.208%
40	14.692	2141	2143	2147	rVB	70903	72817	2.66%	0.321%
41	14.909	2177	2180	2183	rBV	189424	253832	9.26%	1.118%
42	14.939	2183	2185	2191	rVB2	152808	171623	6.26%	0.756%
43	15.204	2227	2230	2236	rBV	112865	139647	5.09%	0.615%
44	15.262	2237	2240	2244	rVV	173932	212816	7.76%	0.937%
45	15.315	2246	2249	2261	rVB	455370	628343	22.91%	2.767%
46	15.698	2312	2314	2319	rVB	57023	62567	2.28%	0.276%
47	16.750	2489	2493	2499	rVB2	76595	138667	5.06%	0.611%
48	17.186	2561	2567	2578	rBV	61693	197865	7.22%	0.871%

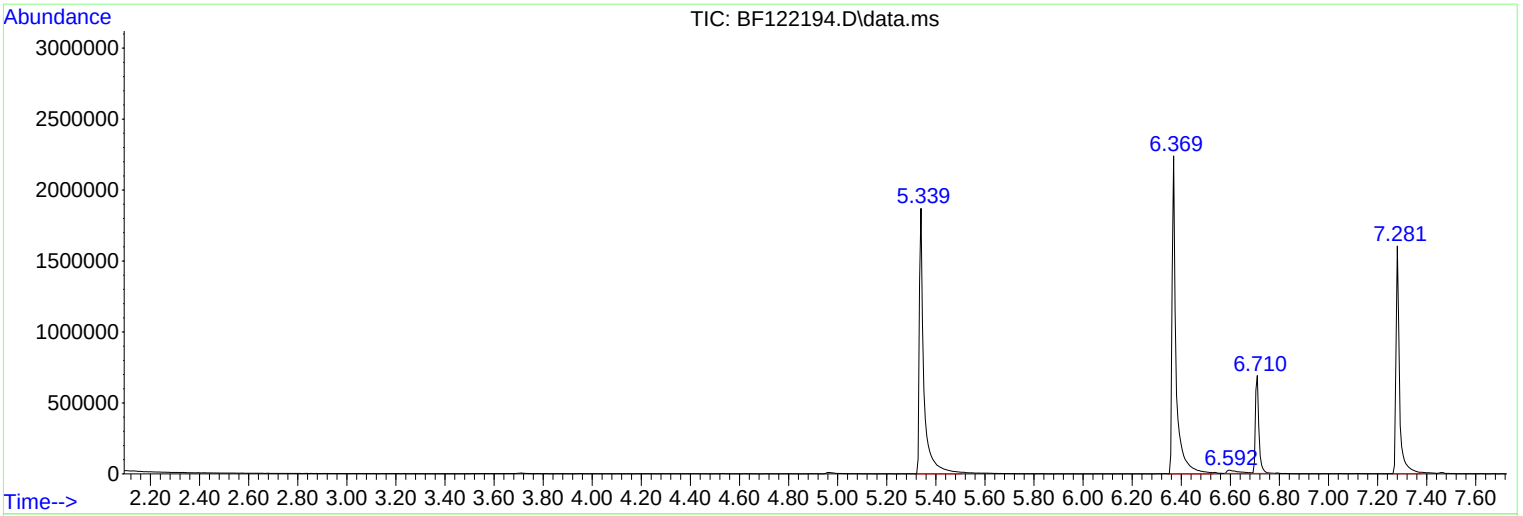
Sum of corrected areas: 22708985

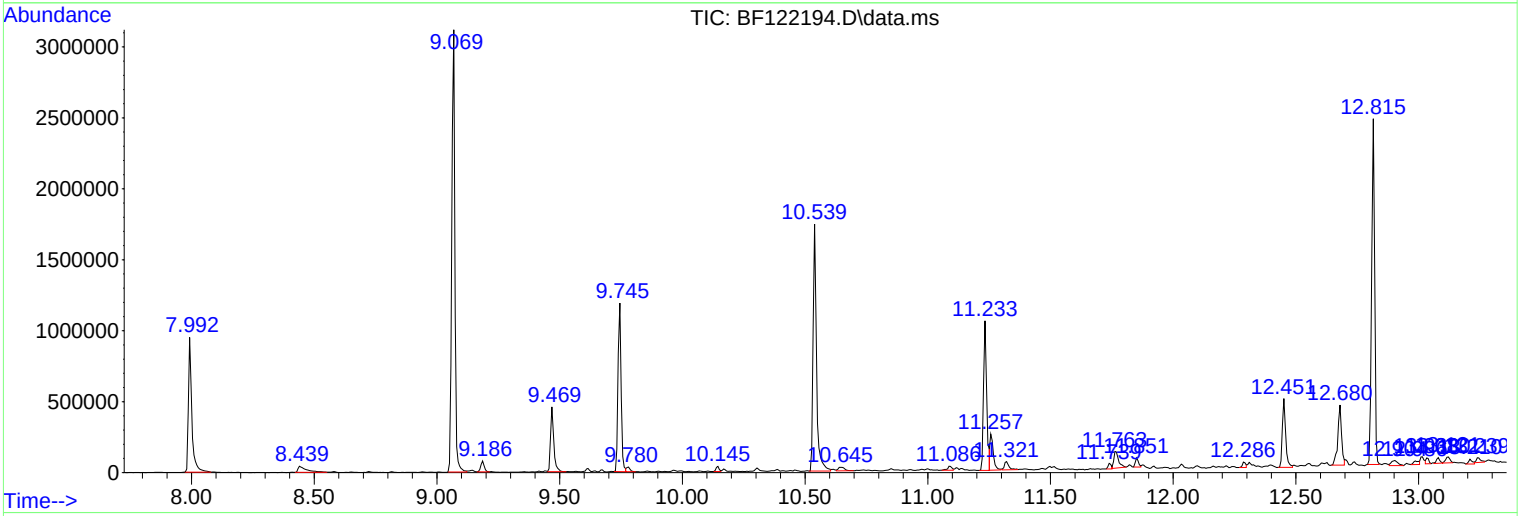
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122194.D
Acq On : 30 Oct 2020 22:23
Operator : JU/CG
Sample : L4565-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

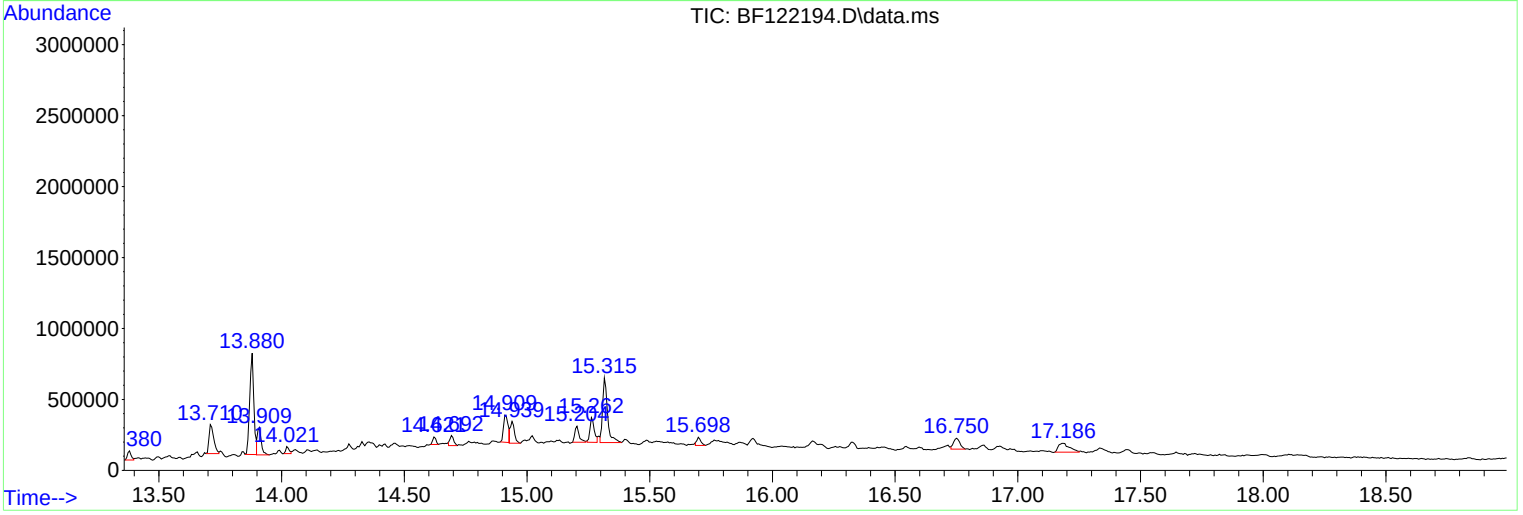
Instrument :
BNA_F
ClientSampleId :
FK-GF-02-063-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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\BF103020\
Data File : BF122194.D
Acq On : 30 Oct 2020 22:23
Operator : JU/CG
Sample : L4565-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-063-A

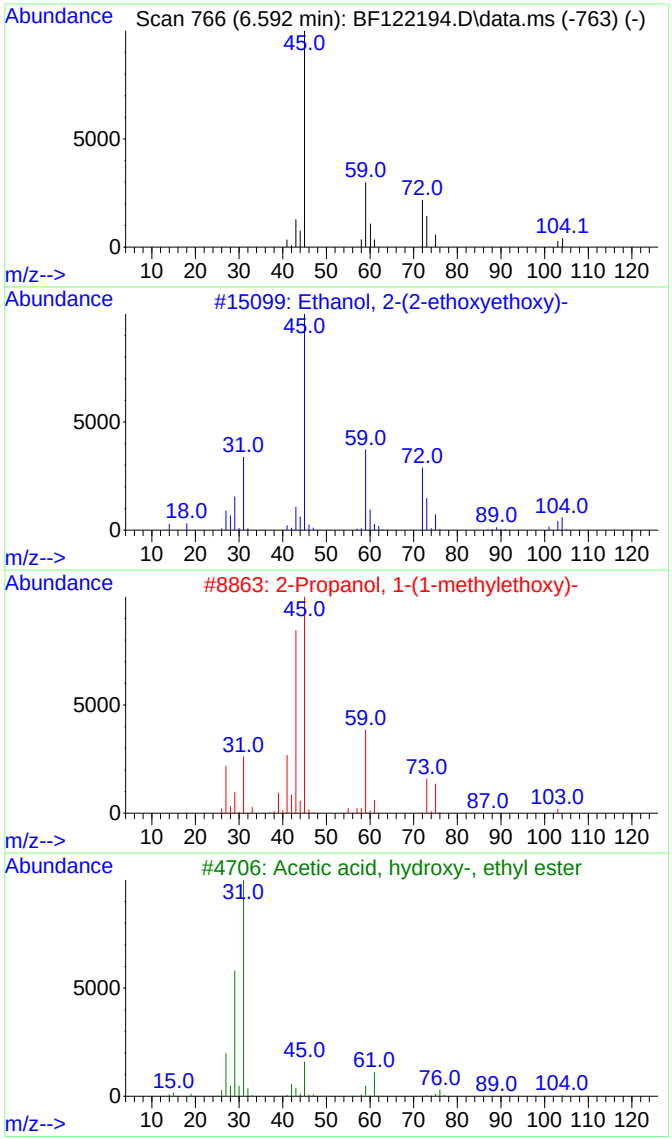
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

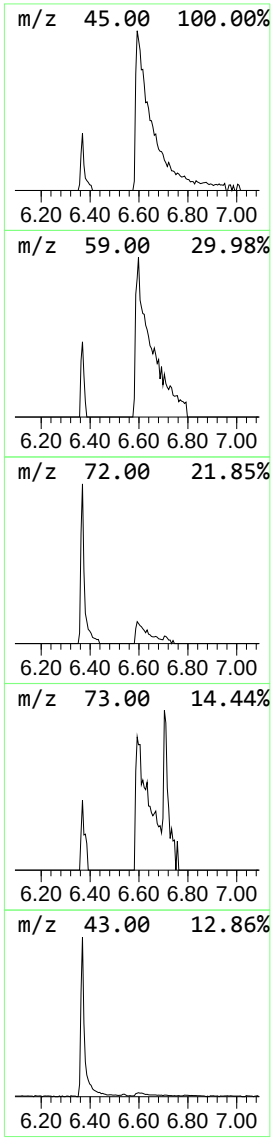
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.592	2.21 ng	75303	1,4-Dichlorobenzene-d4	6.710

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	36
3	Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	9
4	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	9
5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122194.D
Acq On : 30 Oct 2020 22:23
Operator : JU/CG
Sample : L4565-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-063-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

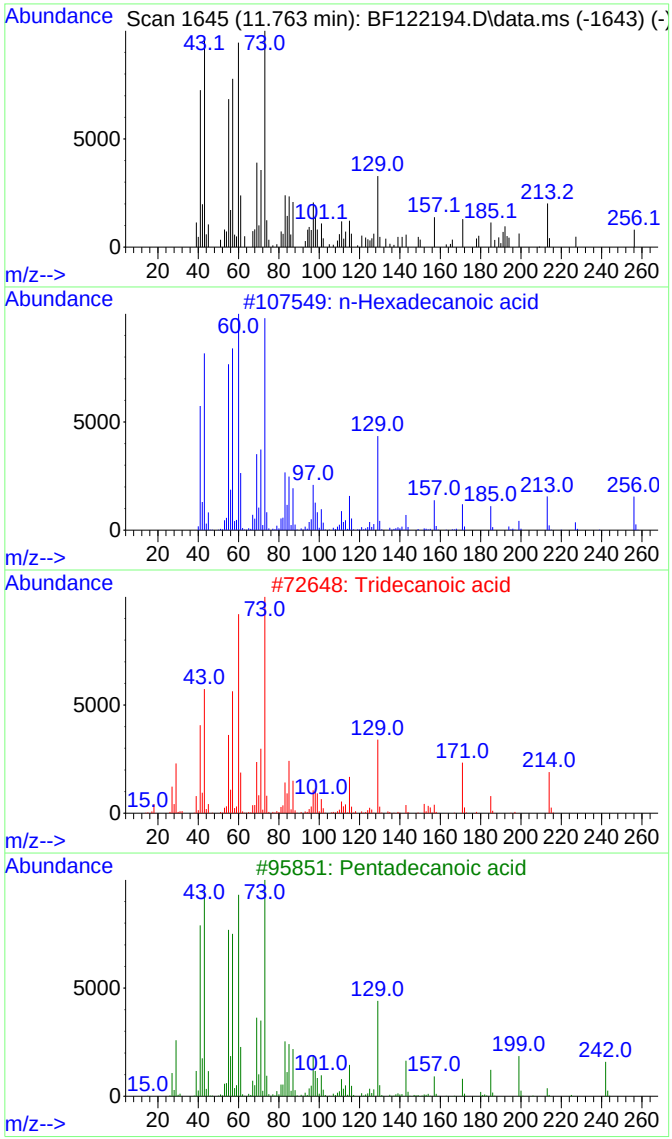
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

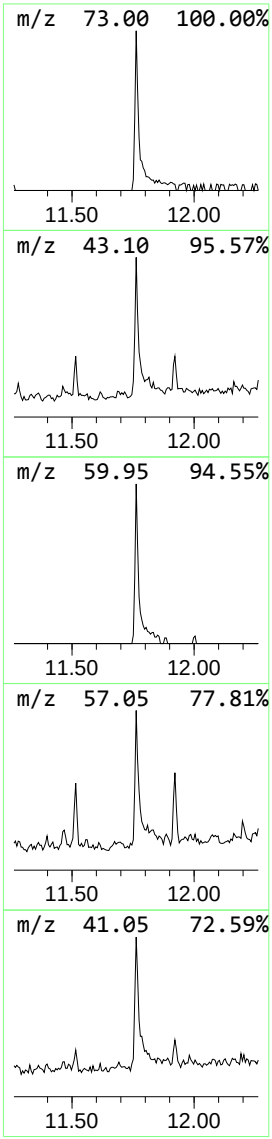
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.763	3.27 ng	155839	Phenanthrene-d10	11.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122194.D
Acq On : 30 Oct 2020 22:23
Operator : JU/CG
Sample : L4565-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-063-A

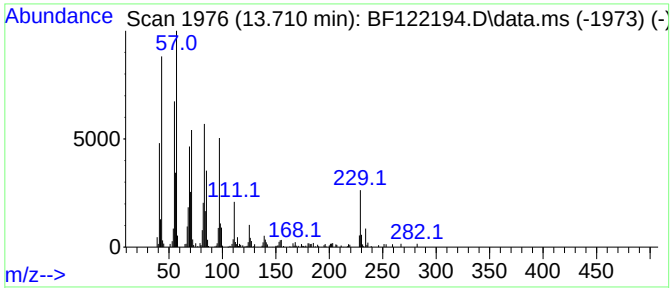
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

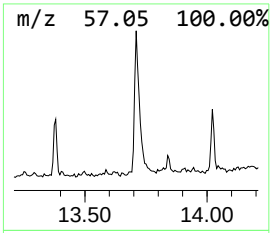
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

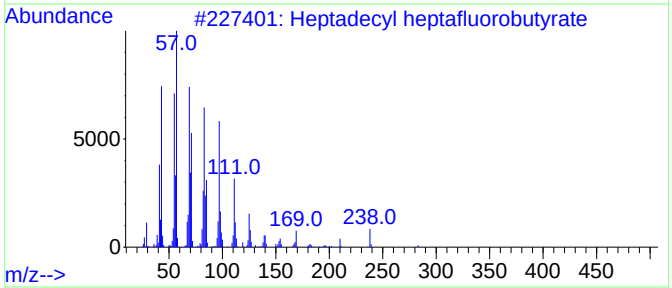
****
Peak Number 3 Heptadecyl heptafluorobutyrate Concentration Rank 1

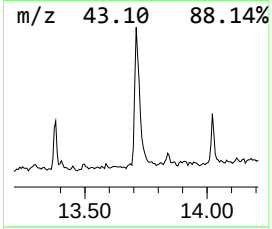
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.710	6.53 ng	274400	Chrysene-d12	13.880

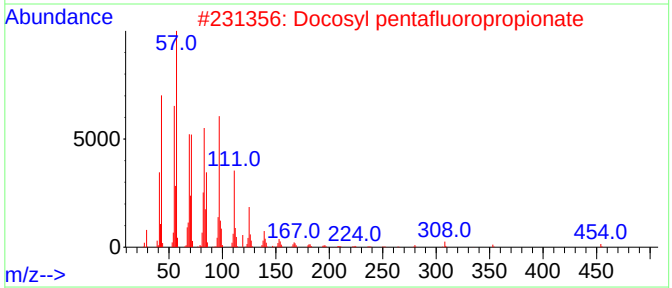
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81
2	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	81
3	17-Pentatriacontene	491	C35H70	006971-40-0	81
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	70
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	64

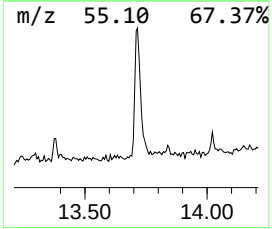


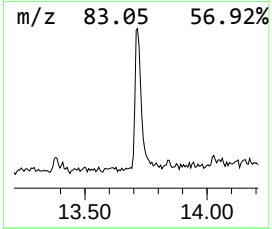


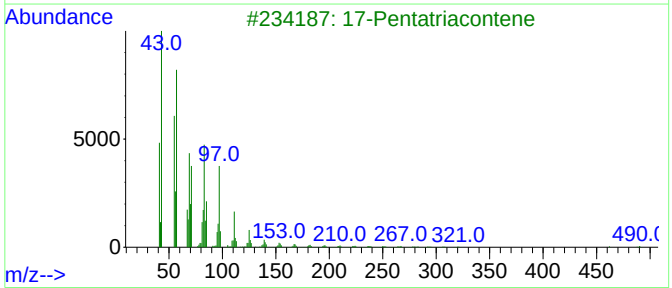


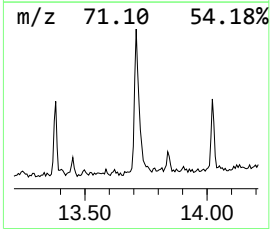












Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122194.D
Acq On : 30 Oct 2020 22:23
Operator : JU/CG
Sample : L4565-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-063-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

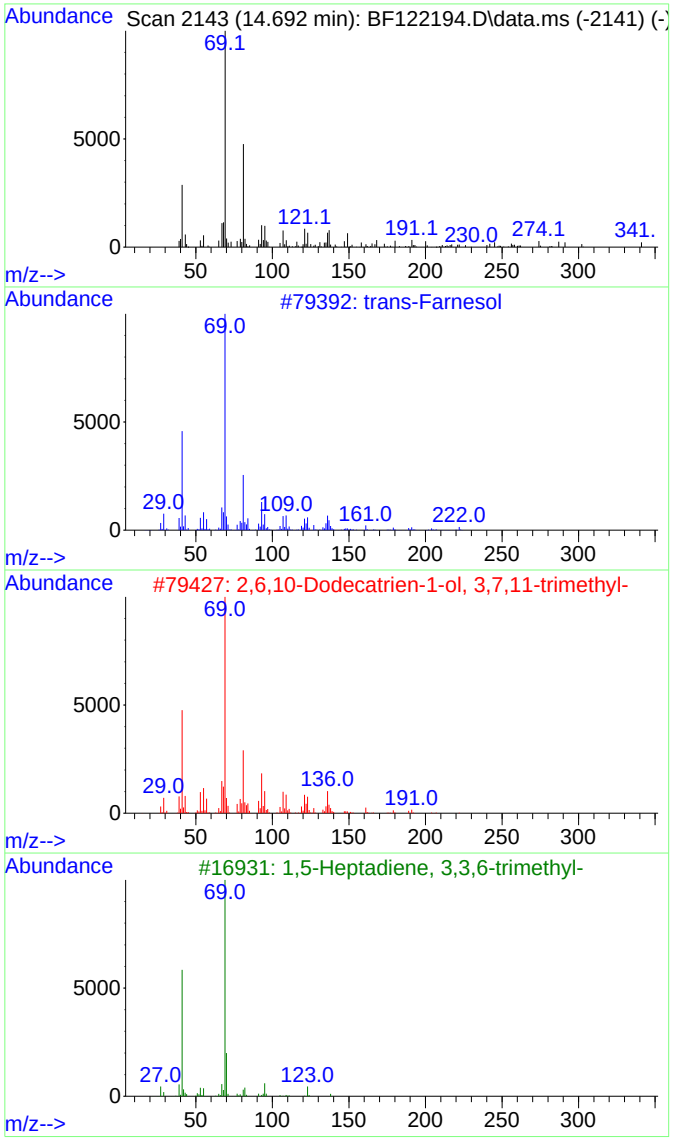
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

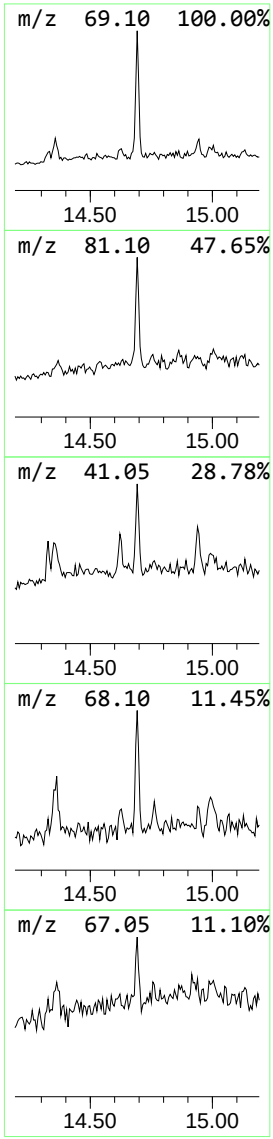
****

Peak Number 4 trans-Farnesol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.692	2.32 ng	72817	Perylene-d12	15.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Farnesol	222	C15H26O	000106-28-5	72
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
3	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	64
4	Squalene	410	C30H50	000111-02-4	64
5	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122194.D
Acq On : 30 Oct 2020 22:23
Operator : JU/CG
Sample : L4565-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FK-GF-02-063-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

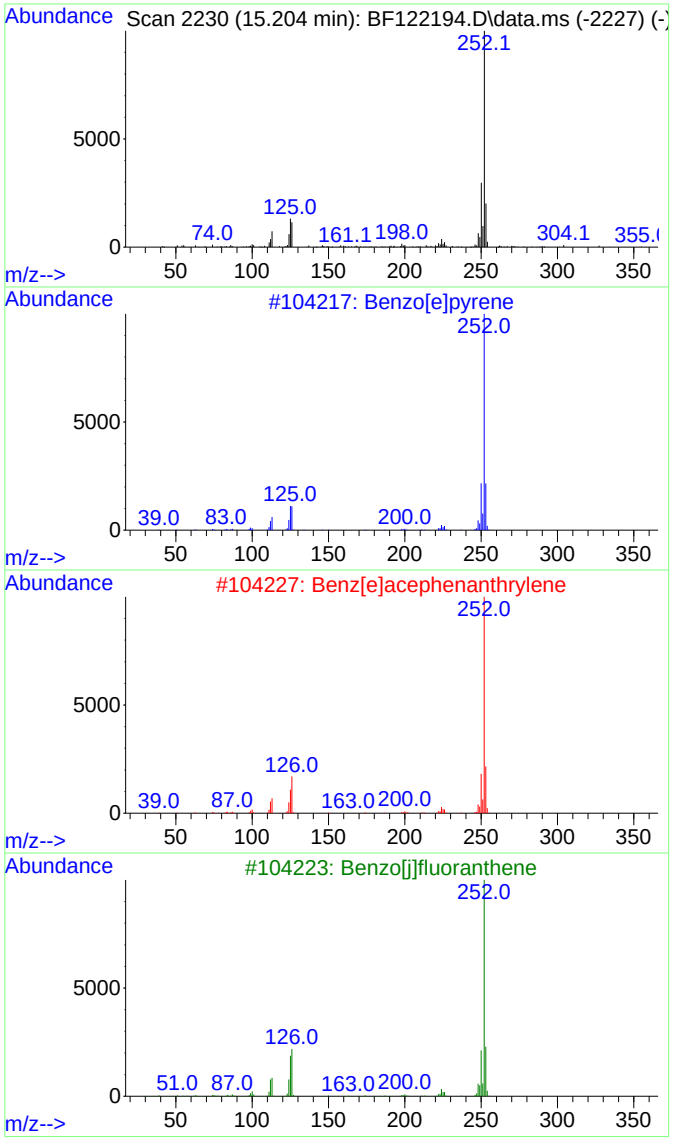
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

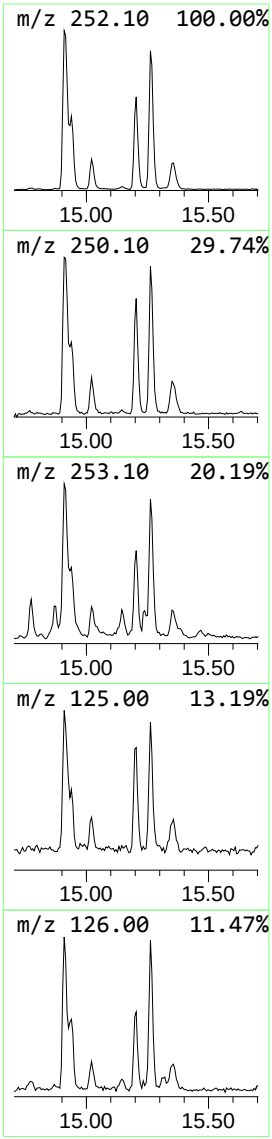
****

Peak Number 5 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.204	4.44 ng	139647	Perylene-d12	15.315

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95
4	Benzo[a]pyrene	252	C20H12	000050-32-8	94
5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF103020\
Data File : BF122194.D
Acq On : 30 Oct 2020 22:23
Operator : JU/CG
Sample : L4565-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-GF-02-063-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101220.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
Ethanol, 2-(2-e...	6.592	2.2	ng	75303	1	6.710	681790	20.0
n-Hexadecanoic ...	11.763	3.3	ng	155839	4	11.233	951703	20.0
Heptadecyl hept...	13.710	6.5	ng	274400	5	13.880	841021	20.0
trans-Farnesol	14.692	2.3	ng	72817	6	15.315	628343	20.0
Benzo[e]pyrene	15.204	4.4	ng	139647	6	15.315	628343	20.0