LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111720\
Data File : BF122349.D
Acq On : 17 Nov 2020 16:49
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-31

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-BF110920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122349.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	5	10	22	rVB	940437	1282879	19.00%	2.281%
2	5.475	571	576	579	rBV	5586281	5581264	82.65%	9.925%
3	6.487	742	748	751	rBV	5238267	5831615	86.35%	10.370%
4	6.687	779	782	788	rBV	191103	167664	2.48%	0.298%
5	6.863	808	812	816	rBV	2047926	1585500	23.48%	2.819%
6	7.422	902	907	911	rBV	3596862	3667599	54.31%	6.522%
7	8.145	1027	1030	1034	rBV	2216167	2034484	30.13%	3.618%
8	9.228	1209	1214	1217	rBV	6874739	6097022	90.28%	10.842%
9	9.345	1227	1234	1245	rVB	357761	396316	5.87%	0.705%
10	9.616	1276	1280	1289	rVB	1376091	1119664	16.58%	1.991%
11	9.904	1325	1329	1333	rBV	2900577	2349742	34.79%	4.178%
12	10.692	1458	1463	1466	rBV	4640070	4395606	65.09%	7.816%
13	11.386	1577	1581	1584	rBV	2682206	2552701	37.80%	4.539%
14	11.410	1584	1585	1588	rVV	637851	410886	6.08%	0.731%
15	11.463	1591	1594	1598	rVB	138737	123410	1.83%	0.219%
16	11.922	1668	1672	1676	rBV	820791	794983	11.77%	1.414%
17	12.004	1682	1686	1688	rBV2	106065	115557	1.71%	0.205%
18	12.174	1712	1715	1718	rBV2	69203	96577	1.43%	0.172%
19	12.204	1718	1720	1726	rVB2	65773	84475	1.25%	0.150%
20	12.374	1745	1749	1754	rBV	229749	214048	3.17%	0.381%
21	12.439	1756	1760	1763	rVV3	96558	134242	1.99%	0.239%
22	12.474	1763	1766	1771	rVB7	48307	81159	1.20%	0.144%
23	12.598	1784	1787	1791	rBV	996671	860425	12.74%	1.530%
24	12.704	1801	1805	1811	rBV3	269344	370827	5.49%	0.659%
25	12.827	1820	1826	1830	rBV	804299	815631	12.08%	1.450%
26	12.980	1847	1852	1855	rBV	6959216	6753168	100.00%	12.009%
27	13.045	1859	1863	1867	rBV3	47968	72320	1.07%	0.129%
28	13.157	1880	1882	1885	rVB	112945	97427	1.44%	0.173%
29	13.221	1885	1893	1896	rBV2	93825	142566	2.11%	0.254%
30	13.263	1896	1900	1903	rVV2	78149	80751	1.20%	0.144%
31	13.663	1965	1968	1972	rVB	64373	68472	1.01%	0.122%
32	13.774	1983	1987	1990	rBV2	68990	85084	1.26%	0.151%
33	13.880	2000	2005	2014	rBV2	495096	758108	11.23%	1.348%
34	14.027	2025	2030	2033	rBV	2549799	2584735	38.27%	4.596%
35	14.051	2033	2034	2040	rVB	375937	258106	3.82%	0.459%
36	14.510	2106	2112	2113	rBV5	76819	106354	1.57%	0.189%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111720\
Data File : BF122349.D
Acq On : 17 Nov 2020 16:49
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-31

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-BF110920.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.892	2174	2177	2188	rVB3	118530	163803	2.43%	0.291%
38	15.068	2202	2207	2210	rBV	284108	456466	6.76%	0.812%
39	15.157	2218	2222	2224	rBV2	71684	106752	1.58%	0.190%
40	15.368	2254	2258	2264	rVB	181181	222179	3.29%	0.395%
41	15.427	2264	2268	2274	rBV	220128	276719	4.10%	0.492%
42	15.498	2274	2280	2284	rBV	1659163	2049565	30.35%	3.645%
43	15.980	2358	2362	2367	rBV	63081	102618	1.52%	0.182%
44	16.051	2370	2374	2386	rVB10	55492	152622	2.26%	0.271%
45	16.786	2494	2499	2507	rVB6	47555	106523	1.58%	0.189%
46	16.951	2522	2527	2535	rVB2	116026	220394	3.26%	0.392%
47	17.386	2597	2601	2615	rVB2	94856	206259	3.05%	0.367%

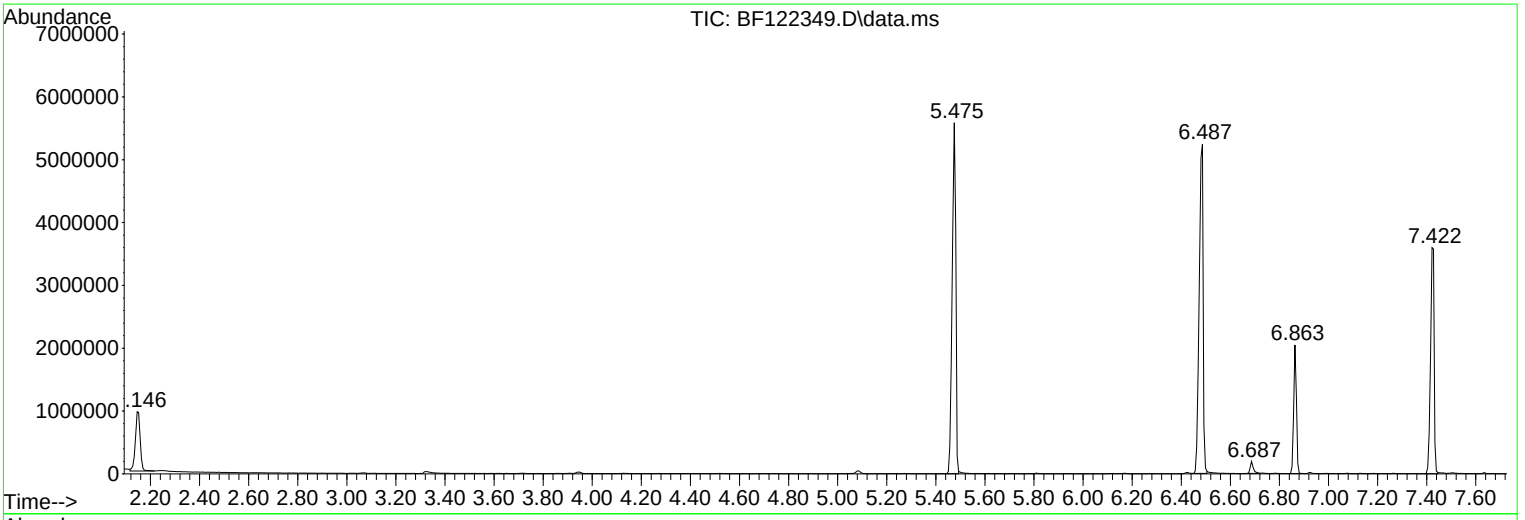
Sum of corrected areas: 56235267

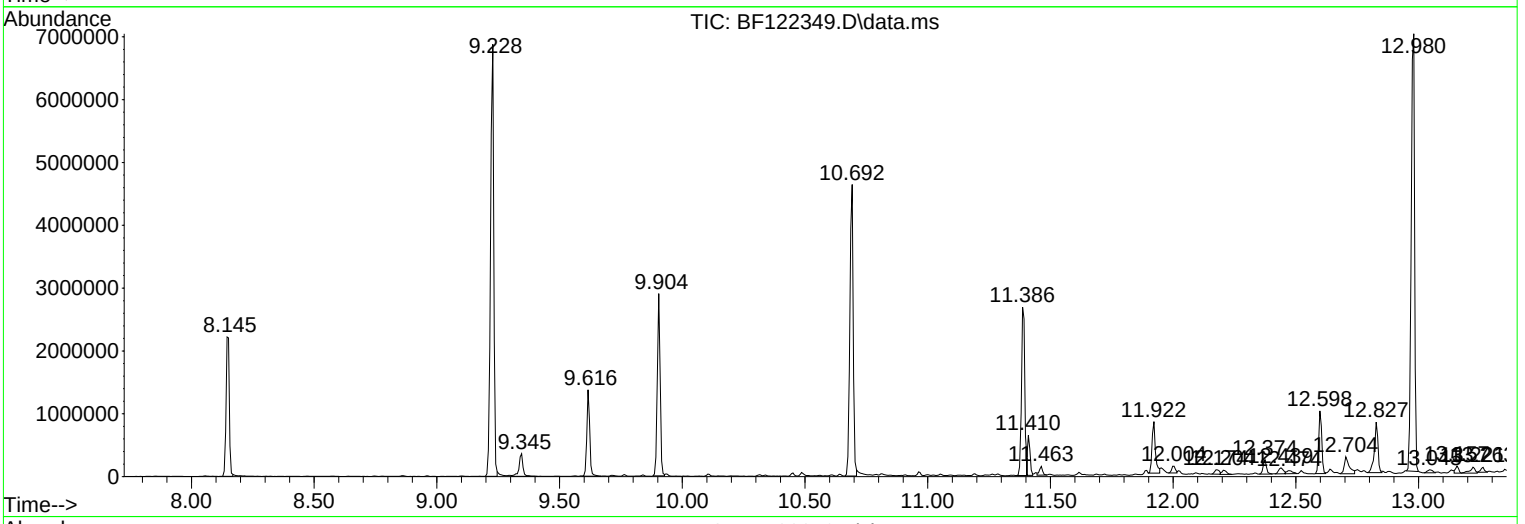
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111720\
Data File : BF122349.D
Acq On : 17 Nov 2020 16:49
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

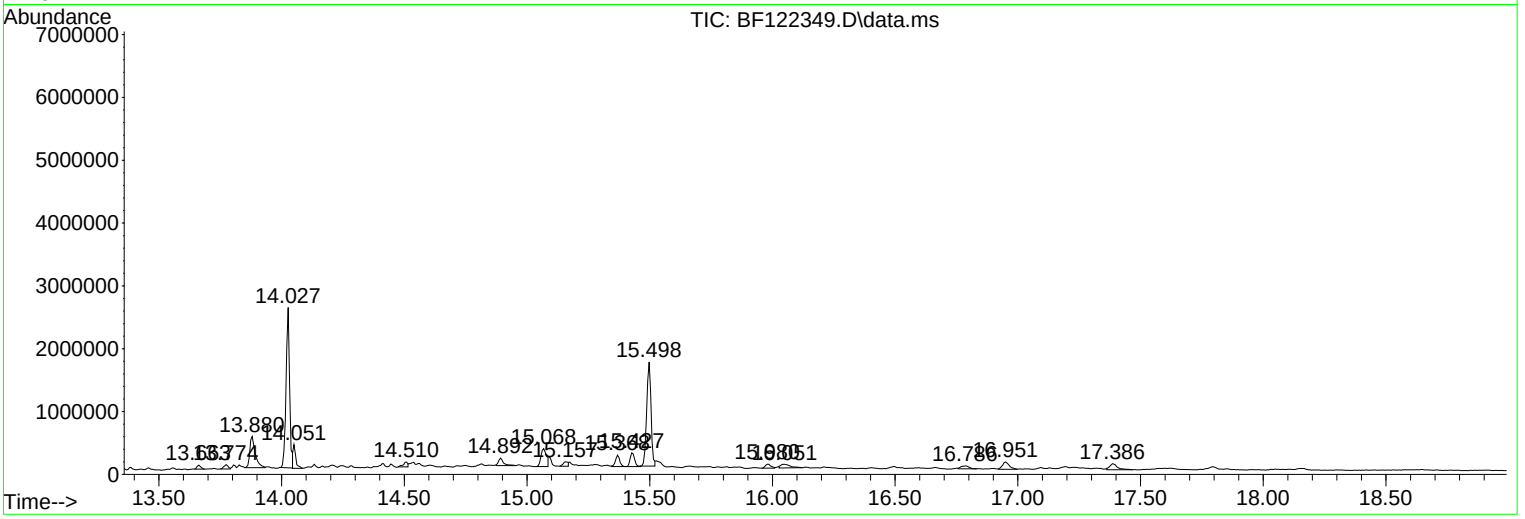
Instrument :
BNA_F
ClientSampleId :
RBR-31

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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\BF111720\
Data File : BF122349.D
Acq On : 17 Nov 2020 16:49
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-31

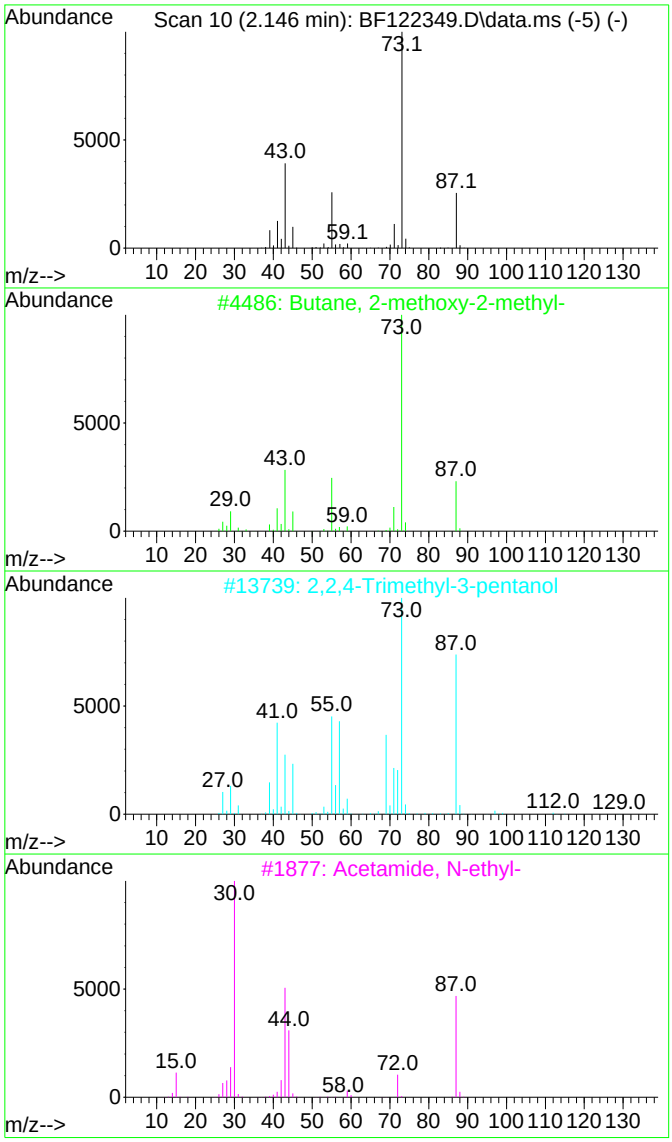
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

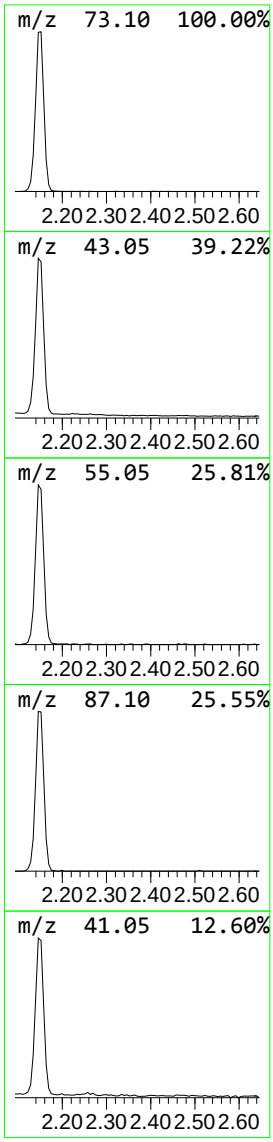
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	16.18 ng	1282880	1,4-Dichlorobenzene-d4	6.863

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111720\
Data File : BF122349.D
Acq On : 17 Nov 2020 16:49
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-31

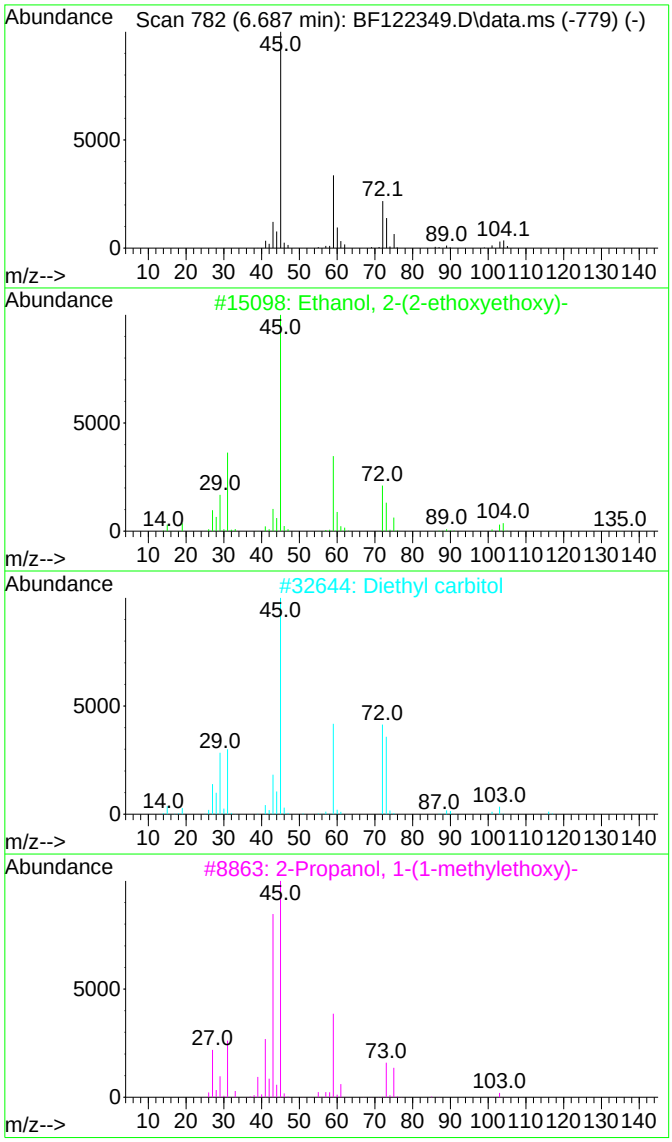
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

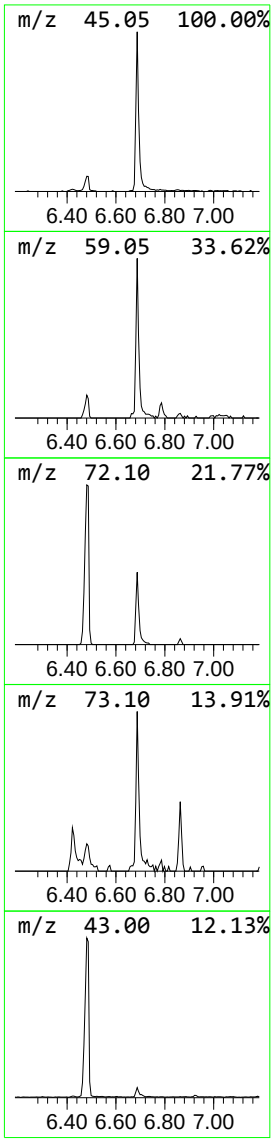
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.687	2.11 ng	167664	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	Diethyl carbitol	162	C8H18O3	000112-36-7	72
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
4	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
5	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111720\
Data File : BF122349.D
Acq On : 17 Nov 2020 16:49
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-31

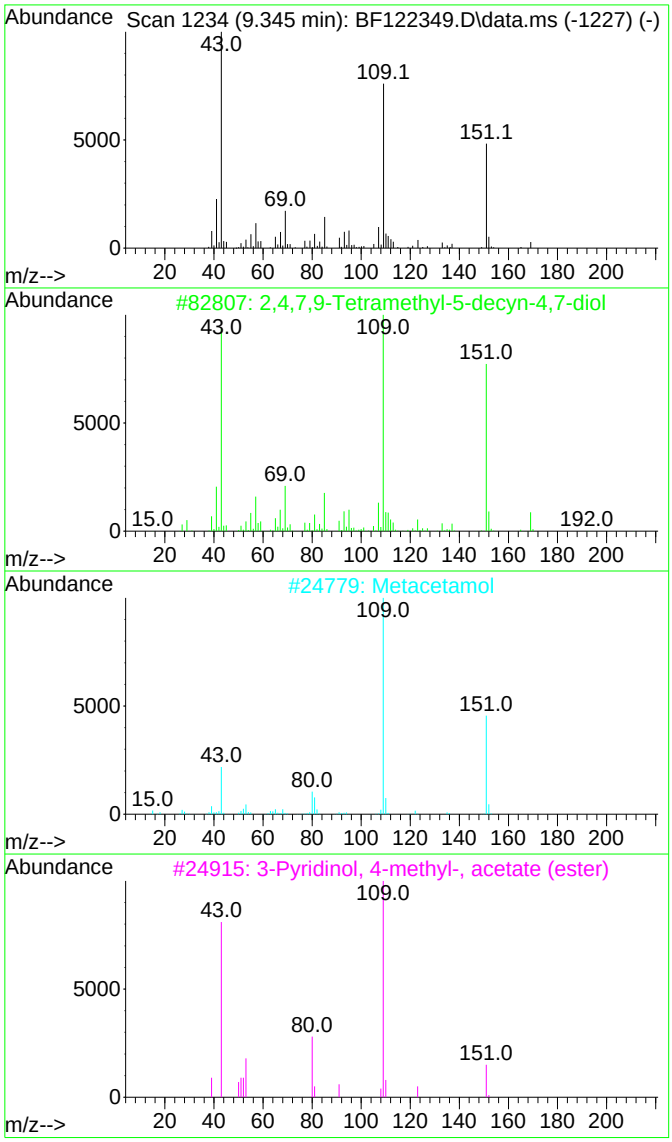
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

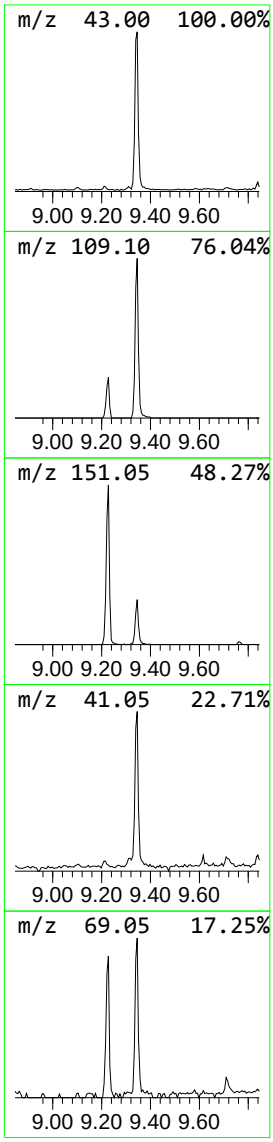
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.345	3.37 ng	396316	Acenaphthene-d10	9.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Metacetamol	151	C8H9NO2	000621-42-1	64
3	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59
4	Acetaminophen	151	C8H9NO2	000103-90-2	59
5	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111720\
Data File : BF122349.D
Acq On : 17 Nov 2020 16:49
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-31

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

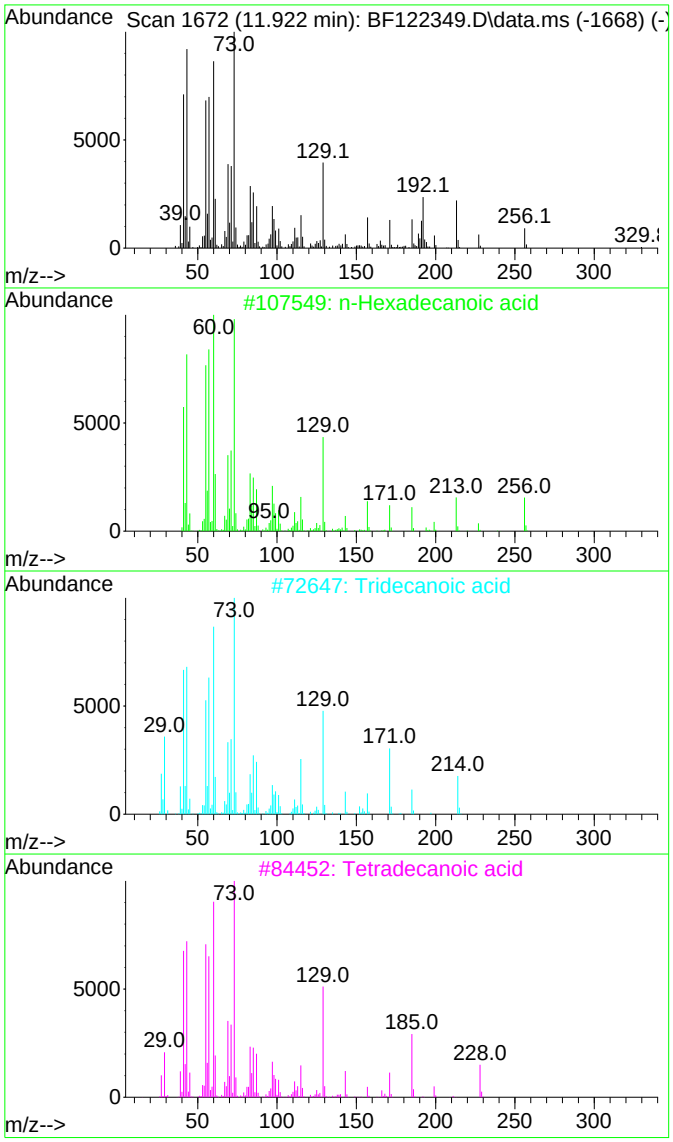
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

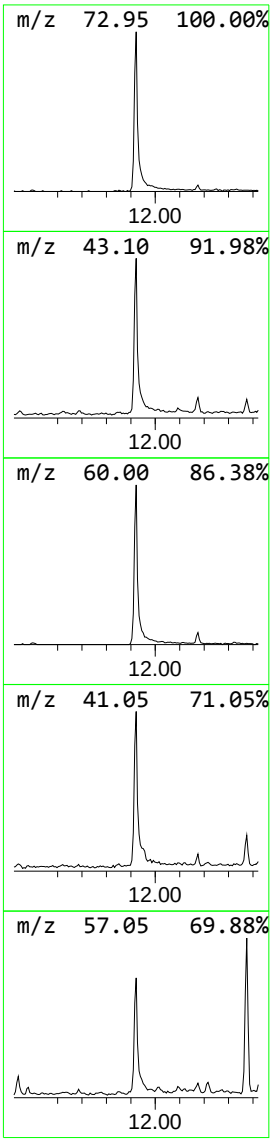
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	6.23 ng	794983	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	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4	Octadecanoic acid	284	C18H36O2	000057-11-4	93
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111720\
Data File : BF122349.D
Acq On : 17 Nov 2020 16:49
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-31

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

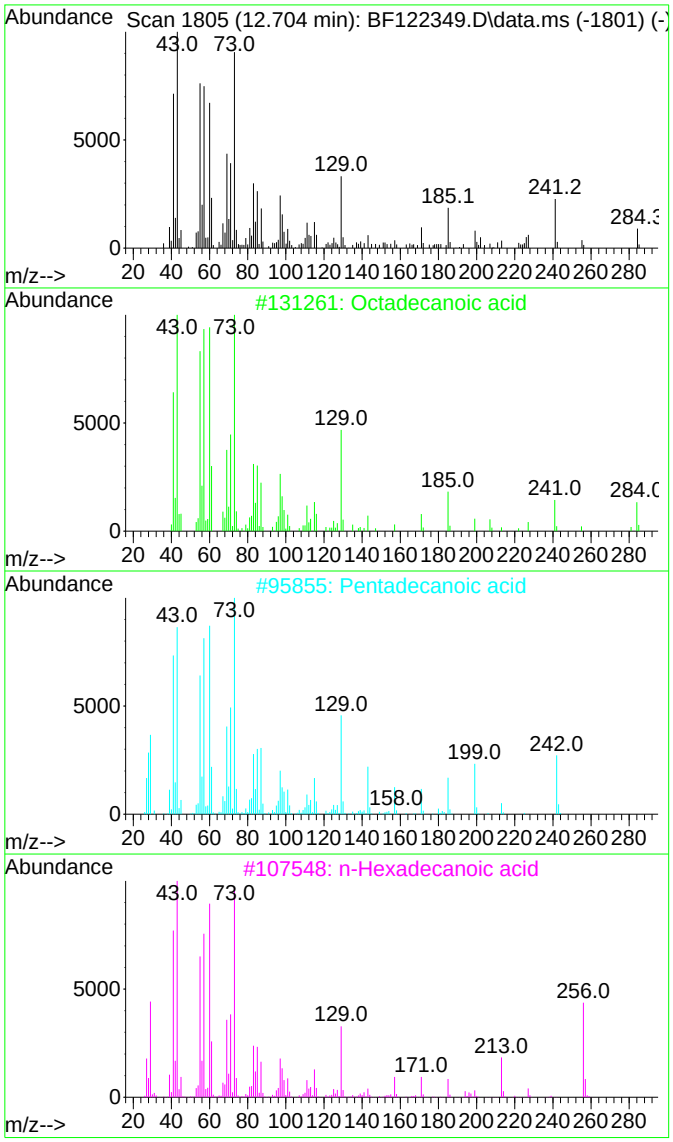
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

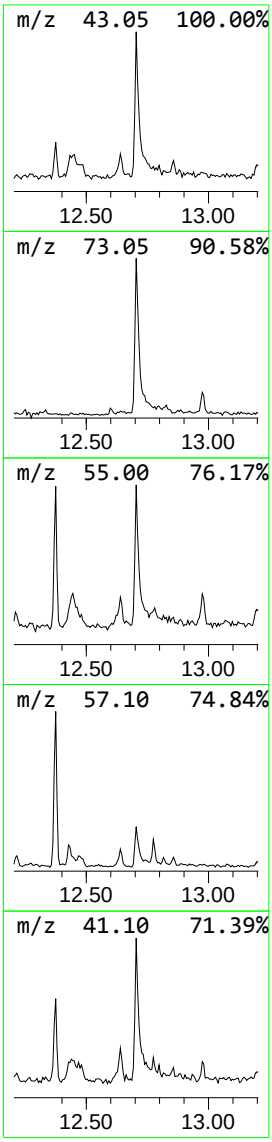
****

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	2.91 ng	370827	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	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111720\
Data File : BF122349.D
Acq On : 17 Nov 2020 16:49
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-31

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

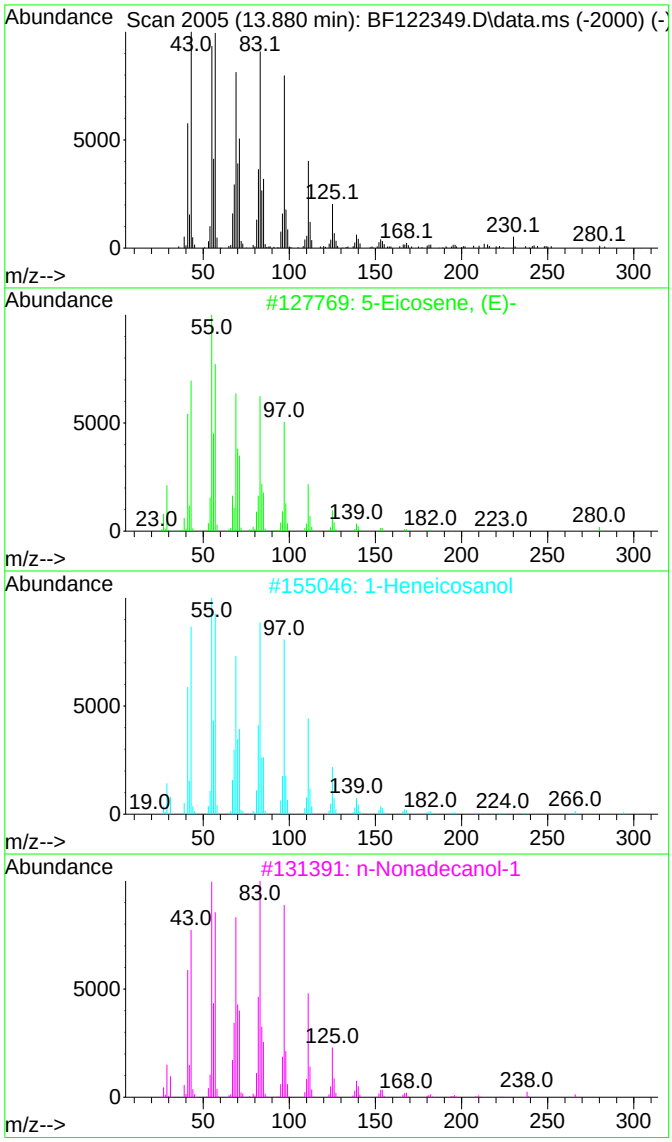
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

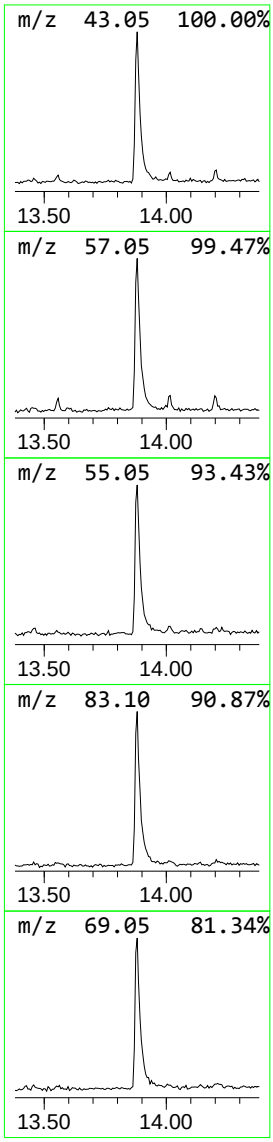
****

Peak Number 6 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	5.87 ng	758108	Chrysene-d12	14.027

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	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111720\
Data File : BF122349.D
Acq On : 17 Nov 2020 16:49
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR-31

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

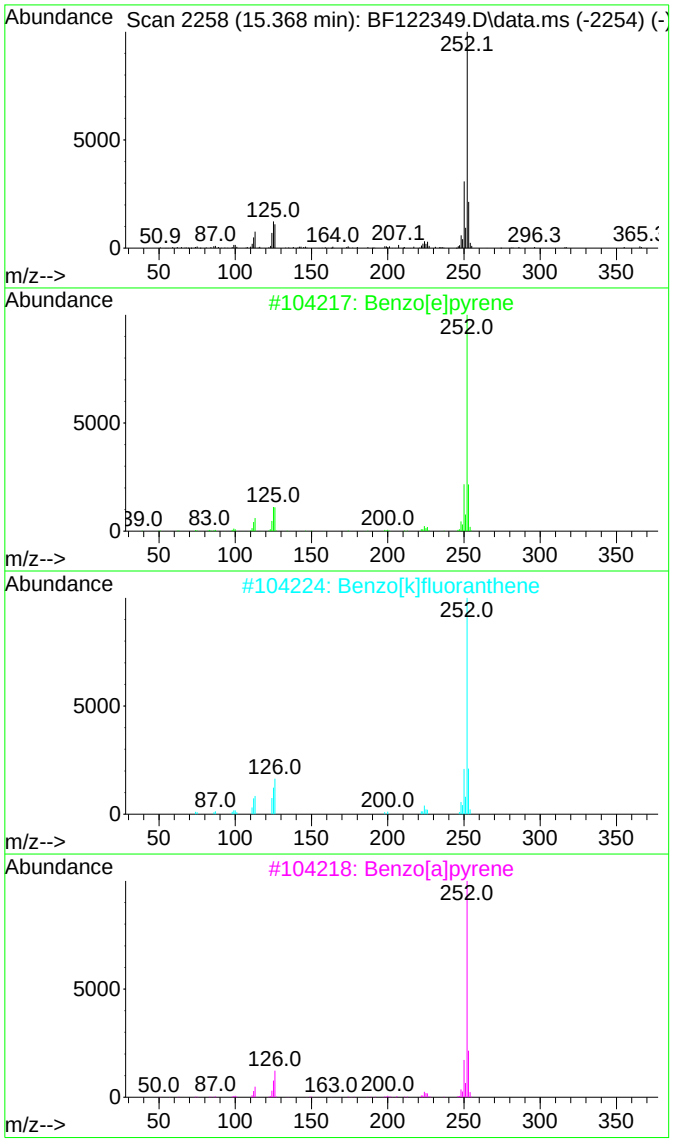
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

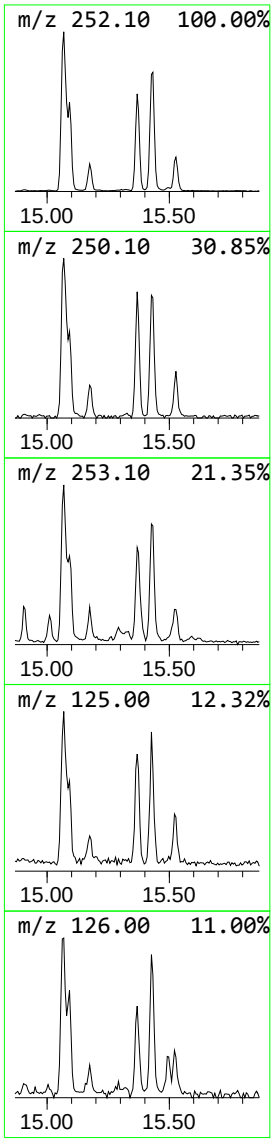
****

Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.368	2.17 ng	222179	Perylene-d12	15.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
3	Benzo[a]pyrene	252	C20H12	000050-32-8	96
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111720\
Data File : BF122349.D
Acq On : 17 Nov 2020 16:49
Operator : JU/CG
Sample : L4725-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RBR-31

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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...	2.146	16.2	ng	1282880	1	6.863	1585500	20.0
Ethanol, 2-(2-e...	6.687	2.1	ng	167664	1	6.863	1585500	20.0
2,4,7,9-Tetrame...	9.345	3.4	ng	396316	3	9.904	2349740	20.0
n-Hexadecanoic ...	11.922	6.2	ng	794983	4	11.386	2552700	20.0
Octadecanoic acid	12.704	2.9	ng	370827	4	11.386	2552700	20.0
5-Eicosene, (E)-	13.880	5.9	ng	758108	5	14.027	2584740	20.0
Benzo[e]pyrene	15.368	2.2	ng	222179	6	15.498	2049570	20.0