LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071823\
Data File : BF134341.D
Acq On : 18 Jul 2023 16:53
Operator : CG\JU
Sample : 03597-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-47-(0-2)

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134341.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	11	rVB	312591	367459	22.34%	2.528%
2	5.087	506	510	515	rBV	22572	32357	1.97%	0.223%
3	5.475	572	576	595	rBV	1784307	1640966	99.76%	11.291%
4	6.481	742	747	763	rBV	1716065	1644849	100.00%	11.318%
5	6.675	776	780	793	rVB	23060	41516	2.52%	0.286%
6	6.840	804	808	815	rBV	607496	514093	31.25%	3.537%
7	7.398	899	903	914	rBV	1174593	1082487	65.81%	7.448%
8	8.116	1021	1025	1028	rBV	876664	671450	40.82%	4.620%
9	9.192	1204	1208	1211	rBV	2150885	1603404	97.48%	11.033%
10	9.304	1224	1227	1231	rBV	26150	25164	1.53%	0.173%
11	9.875	1320	1324	1327	rBV	764892	610824	37.14%	4.203%
12	10.669	1455	1459	1462	rBV	1364834	1116876	67.90%	7.685%
13	11.369	1574	1578	1580	rBV	740359	601519	36.57%	4.139%
14	11.392	1580	1582	1587	rVV	144379	118042	7.18%	0.812%
15	11.445	1587	1591	1594	rVB2	21005	26040	1.58%	0.179%
16	11.898	1665	1668	1675	rBV2	279808	253434	15.41%	1.744%
17	12.592	1782	1786	1789	rBV	237797	211854	12.88%	1.458%
18	12.686	1800	1802	1808	rBV2	74929	85507	5.20%	0.588%
19	12.822	1819	1825	1829	rBV	192392	193041	11.74%	1.328%
20	12.963	1841	1849	1853	rBV	1411362	1285857	78.17%	8.848%
21	13.039	1858	1862	1867	rBV4	15622	27723	1.69%	0.191%
22	13.127	1874	1877	1880	rBV3	14677	24050	1.46%	0.165%
23	13.257	1896	1899	1906	rVB3	22514	25961	1.58%	0.179%
24	13.539	1943	1947	1949	rBV3	23308	27091	1.65%	0.186%
25	13.669	1966	1969	1973	rVB	27460	25659	1.56%	0.177%
26	13.774	1984	1987	1990	rBV	21002	22393	1.36%	0.154%
27	13.874	2001	2004	2005	rBV	26004	28958	1.76%	0.199%
28	13.898	2005	2008	2015	rVB4	41413	77962	4.74%	0.536%
29	14.027	2022	2030	2033	rBV2	478782	596003	36.23%	4.101%
30	14.057	2033	2035	2041	rVV	105694	106474	6.47%	0.733%
31	14.121	2042	2046	2051	rVV	182096	184087	11.19%	1.267%
32	14.186	2054	2057	2064	rVV3	26435	43944	2.67%	0.302%
33	14.421	2094	2097	2100	rVB	25320	22624	1.38%	0.156%
34	14.498	2106	2110	2114	rBV3	36939	47676	2.90%	0.328%
35	15.092	2207	2211	2214	rBV	101694	150029	9.12%	1.032%
36	15.157	2219	2222	2227	rVB2	40048	54067	3.29%	0.372%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071823\
Data File : BF134341.D
Acq On : 18 Jul 2023 16:53
Operator : CG\JU
Sample : 03597-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-47-(0-2)

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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.404	2261	2264	2269	rVB	60348	77472	4.71%	0.533%
38	15.468	2272	2275	2281	rVV	85018	103733	6.31%	0.714%
39	15.539	2282	2287	2300	rVB	420375	605149	36.79%	4.164%
40	16.545	2456	2458	2464	rBV7	18823	31564	1.92%	0.217%
41	17.074	2544	2548	2559	rBV3	45374	123785	7.53%	0.852%

Sum of corrected areas: 14533143

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071823\
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Acq On : 18 Jul 2023 16:53
Operator : CG\JU
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Misc :
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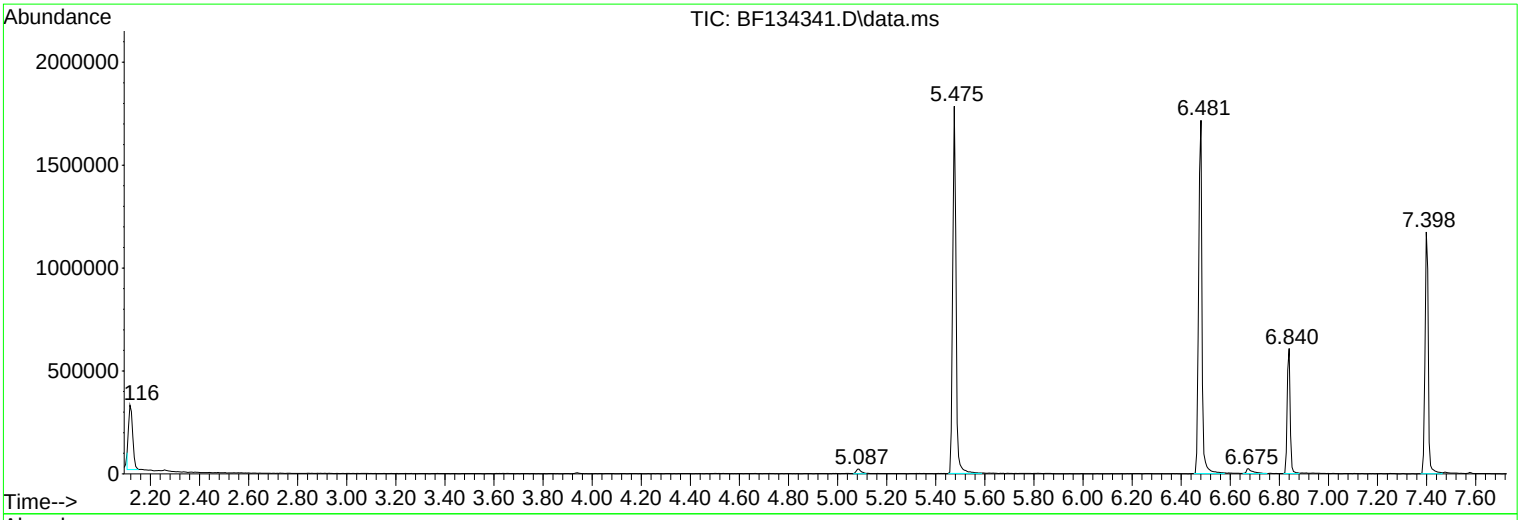
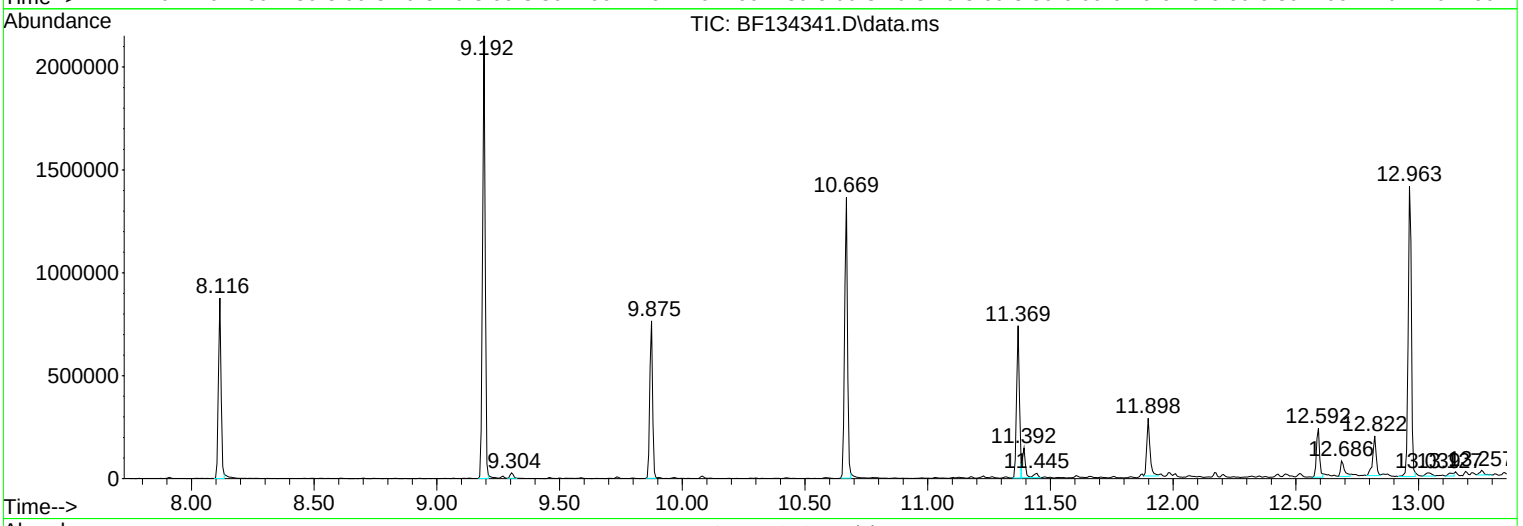
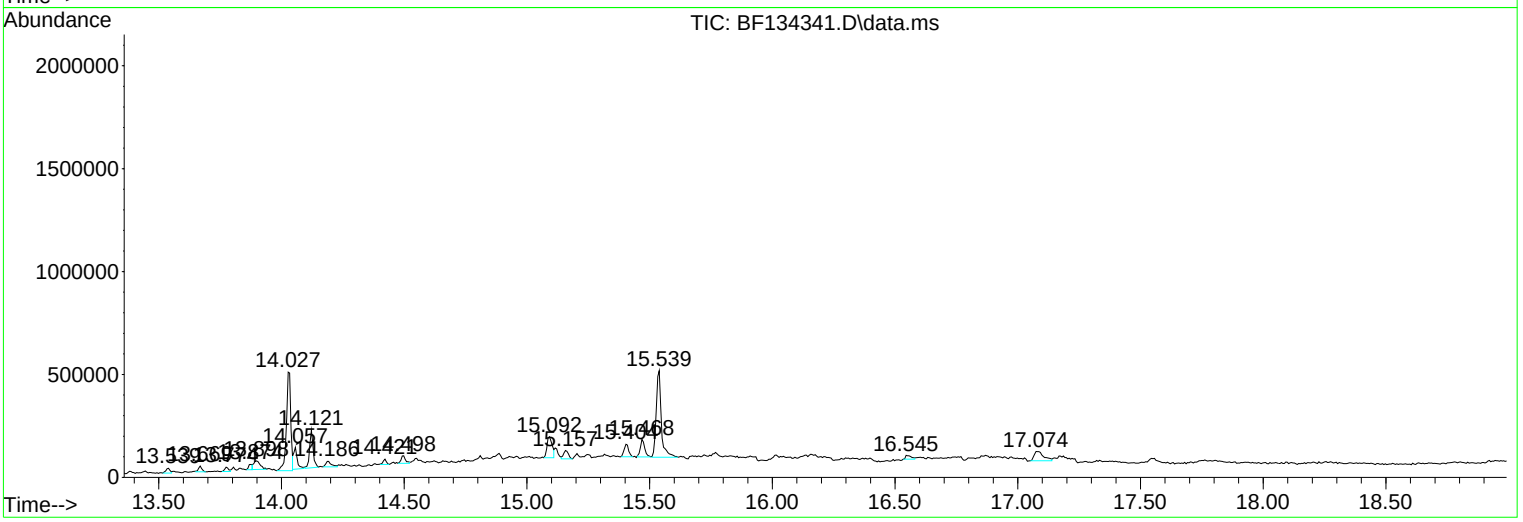
Instrument :
BNA_F
ClientSampleId :
RB-47-(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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Data File : BF134341.D
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Operator : CG\JU
Sample : 03597-11
Misc :
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Instrument :
BNA_F
ClientSampleId :
RB-47-(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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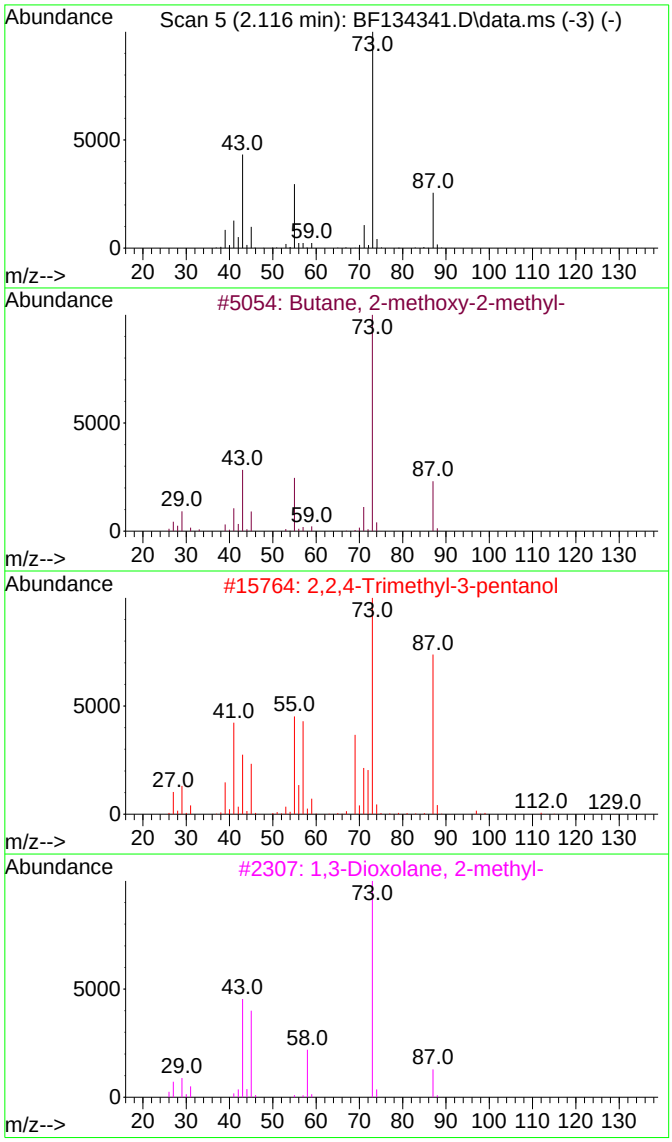
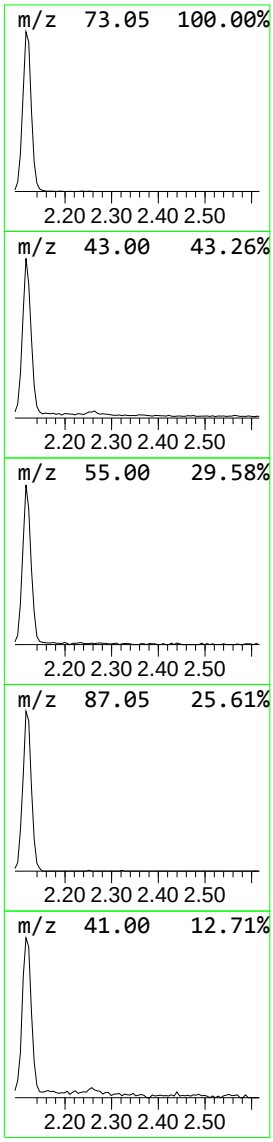
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	14.30 ng	367459	1,4-Dichlorobenzene-d4	6.840

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	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





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Data File : BF134341.D
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Operator : CG\JU
Sample : 03597-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-47-(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

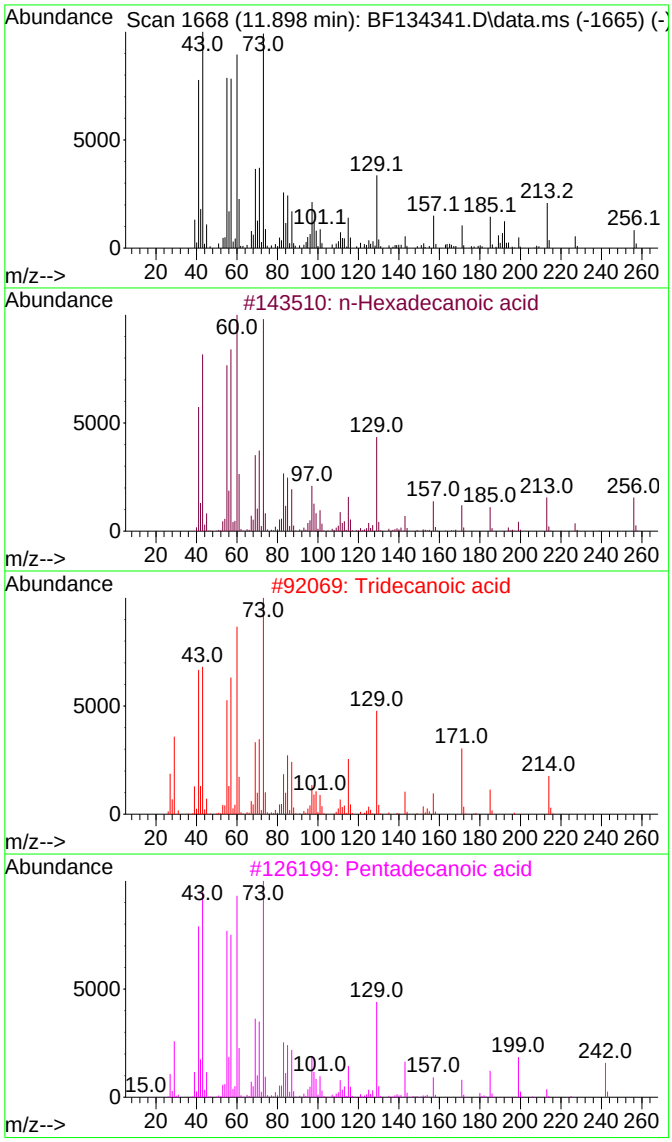
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

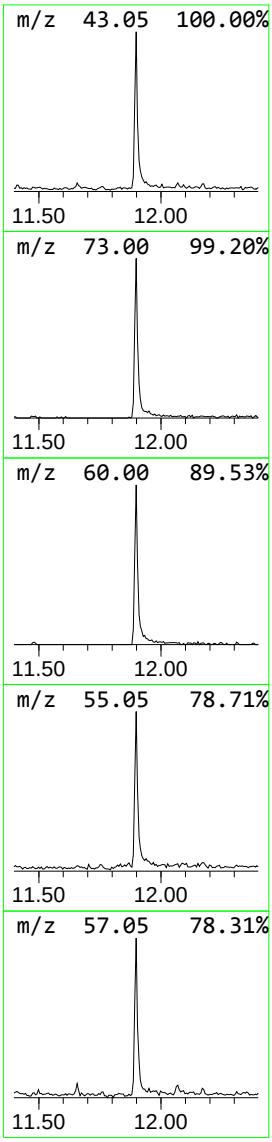
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	8.43 ng	253434	Phenanthrene-d10	11.369

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071823\
Data File : BF134341.D
Acq On : 18 Jul 2023 16:53
Operator : CG\JU
Sample : 03597-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-47-(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

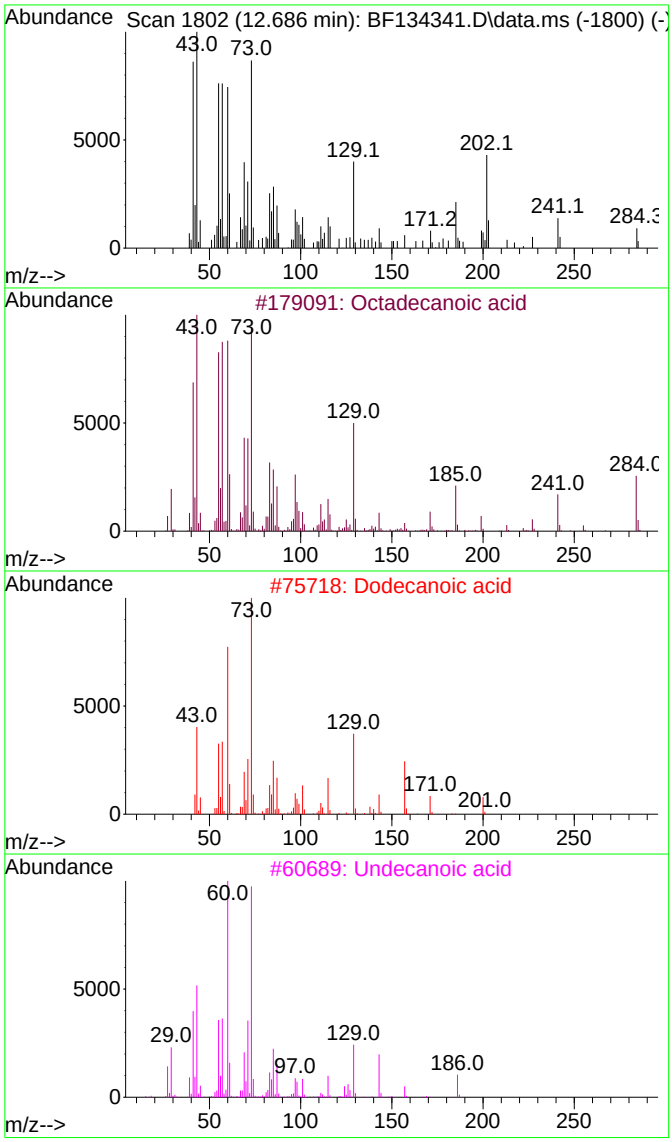
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

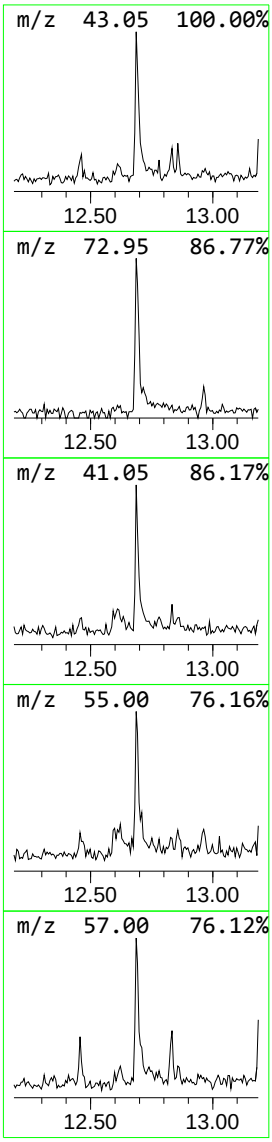
****

Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.686	2.84 ng	85507	Phenanthrene-d10	11.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Dodecanoic acid	200	C12H24O2	000143-07-7	91
3	Undecanoic acid	186	C11H22O2	000112-37-8	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071823\
Data File : BF134341.D
Acq On : 18 Jul 2023 16:53
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-47-(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

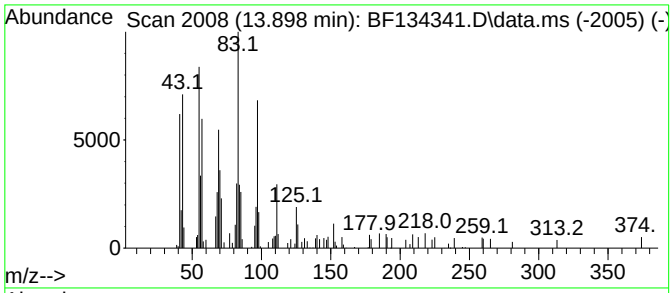
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

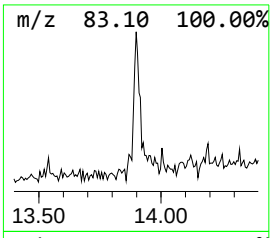
****

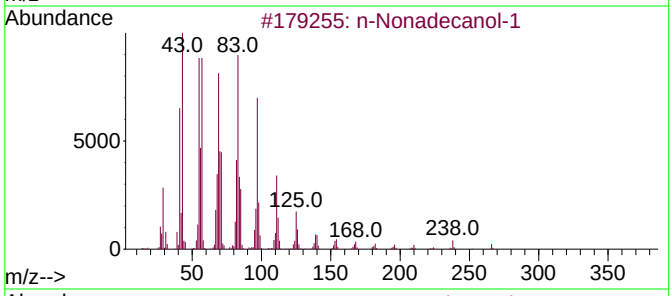
Peak Number 4 n-Nonadecanol-1 Concentration Rank 6

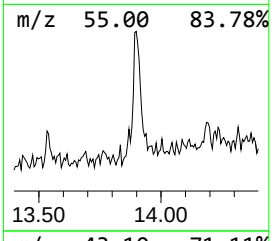
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	2.62 ng	77962	Chrysene-d12	14.033

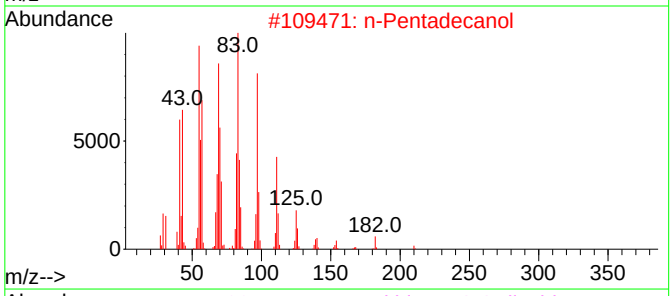
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	58
2	n-Pentadecanol	228	C15H32O	000629-76-5	53
3	4-n-Hexylthiane, S,S-dioxide	218	C11H22O2S	070928-52-8	53
4	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	52
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	52

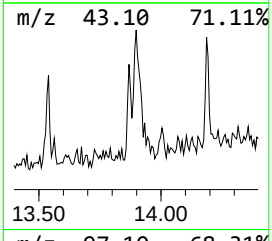


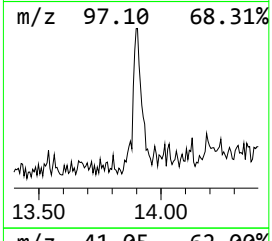


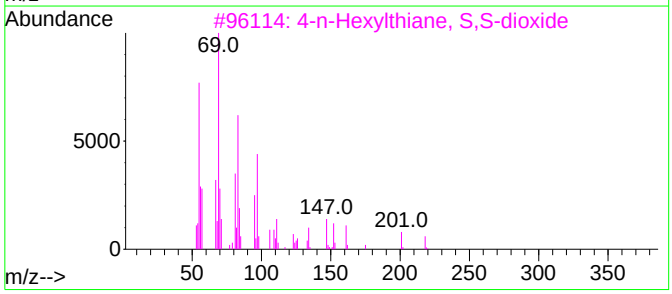


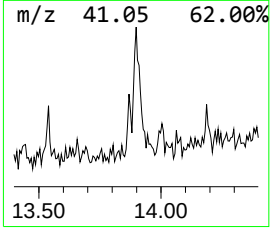












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Misc :
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Instrument :
BNA_F
ClientSampleId :
RB-47-(0-2)

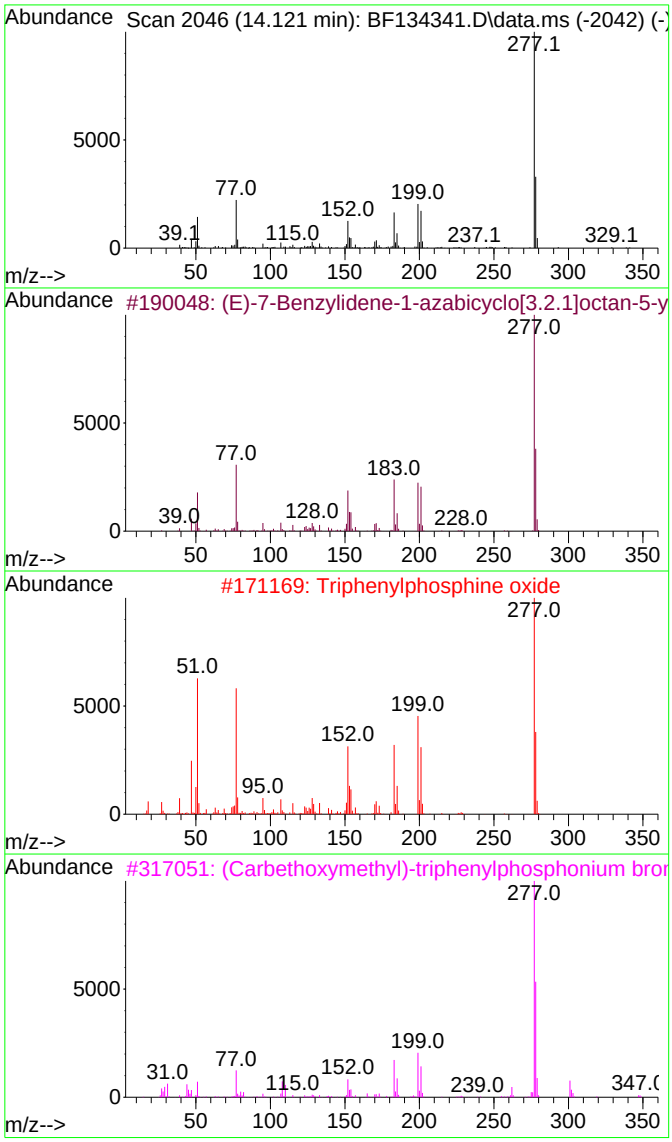
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

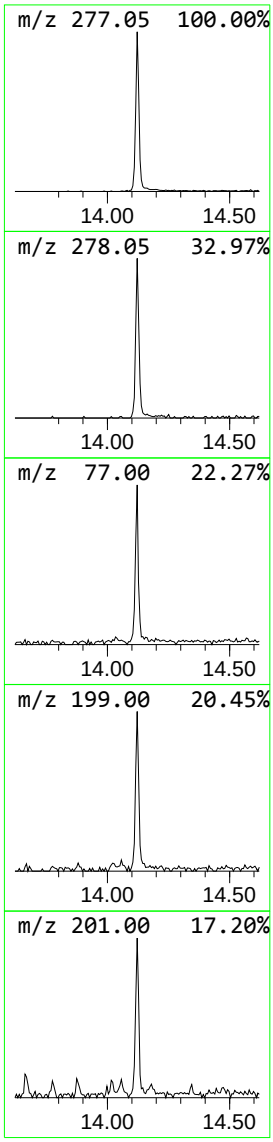
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (E)-7-Benzylidene-1-azabicy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.121	6.18 ng	184087	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	70
3	(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	64
4	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	45
5	Thiophene-3-carbonitrile, 4-(4-m...	277	C13H11NO2S2	1000268-75-0	43





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

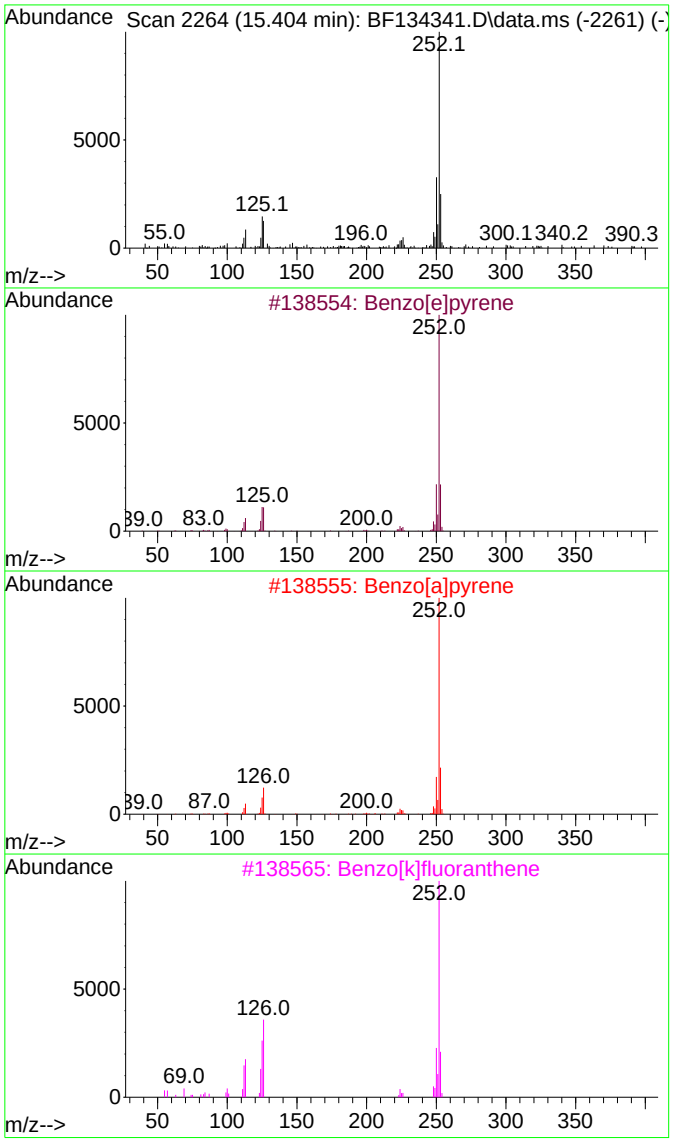
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

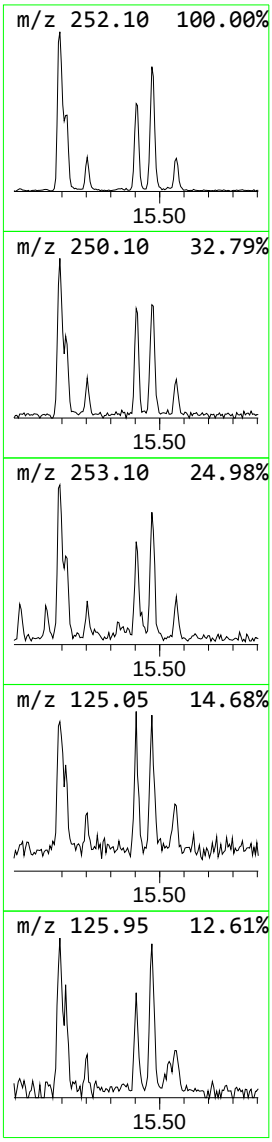
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.404	2.56 ng	77472	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[a]pyrene	252	C20H12	000050-32-8	96
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071823\
Data File : BF134341.D
Acq On : 18 Jul 2023 16:53
Operator : CG\JU
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Misc :
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Instrument :
BNA_F
ClientSampleId :
RB-47-(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

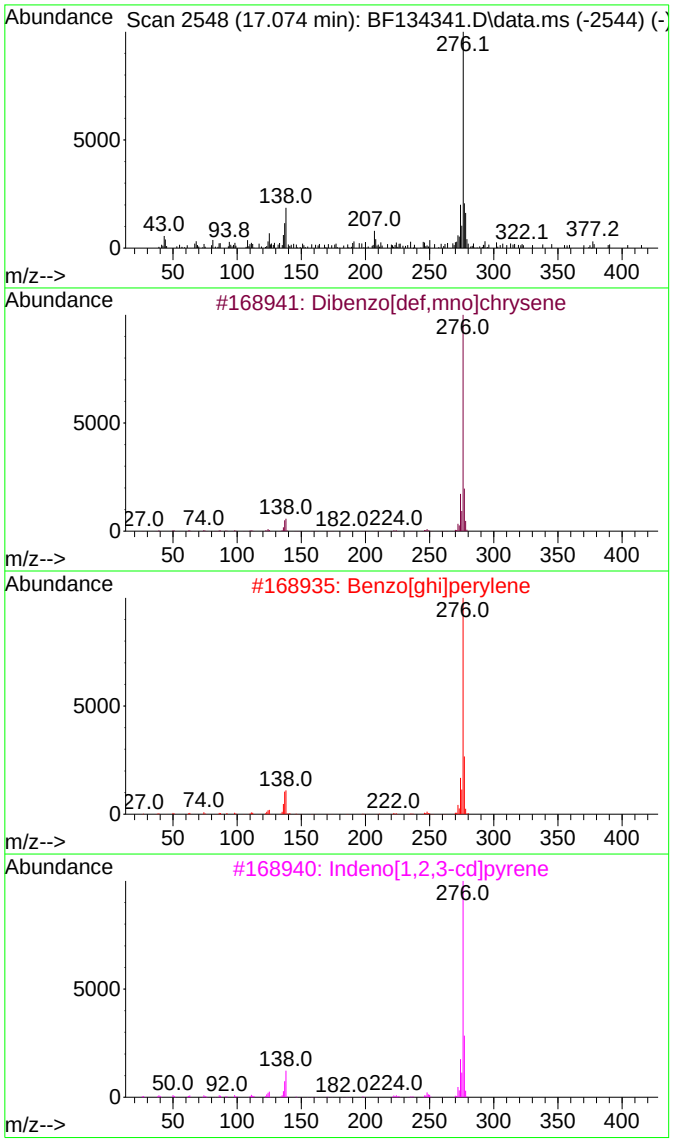
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

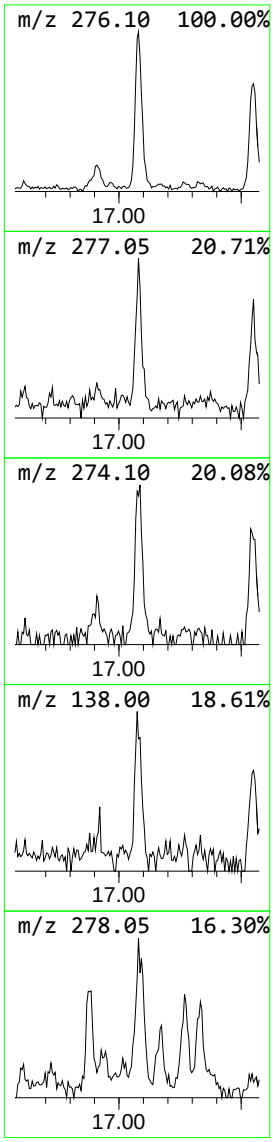
****

Peak Number 7 Dibenzo[def,mno]chrysene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.074	4.09 ng	123785	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	76
2	Benzo[ghi]perylene	276	C22H12	000191-24-2	70
3	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	62
4	6-Amino-3-methylanthrapyridine	276	C17H12N2O2	014642-72-9	58
5	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071823\
Data File : BF134341.D
Acq On : 18 Jul 2023 16:53
Operator : CG\JU
Sample : 03597-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RB-47-(0-2)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.116	14.3	ng	367459	1	6.840	514093	20.0
n-Hexadecanoic ...	11.898	8.4	ng	253434	4	11.369	601519	20.0
Octadecanoic acid	12.686	2.8	ng	85507	4	11.369	601519	20.0
n-Nonadecanol-1	13.898	2.6	ng	77962	5	14.033	596003	20.0
(E)-7-Benzylide...	14.121	6.2	ng	184087	5	14.033	596003	20.0
Benzo[e]pyrene	15.404	2.6	ng	77472	6	15.539	605149	20.0
Dibenzo[def,mno...	17.074	4.1	ng	123785	6	15.539	605149	20.0