LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080322\
Data File : BF129550.D
Acq On : 03 Aug 2022 20:31
Operator : CG\JU
Sample : N3930-20
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RVE-112

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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129550.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.104	476	479	487	rBV	47023	61916	1.66%	0.191%
2	5.504	543	547	550	rBV	4054158	3591500	96.37%	11.057%
3	6.516	714	719	722	rBV	3756782	3469012	93.08%	10.680%
4	6.869	775	779	782	rBV	1042095	815738	21.89%	2.511%
5	7.434	870	875	878	rBV	2515864	2253484	60.47%	6.938%
6	8.151	993	997	1000	rBV	1260839	998768	26.80%	3.075%
7	9.228	1175	1180	1183	rBV	4090772	3726781	100.00%	11.474%
8	9.557	1232	1236	1240	rBV2	111305	91813	2.46%	0.283%
9	9.904	1292	1295	1299	rBV	1088221	966280	25.93%	2.975%
10	10.669	1422	1425	1427	rBV	301901	242503	6.51%	0.747%
11	10.698	1427	1430	1439	rVB	2163850	1817299	48.76%	5.595%
12	11.398	1545	1549	1551	rBV	853042	768294	20.62%	2.365%
13	11.422	1551	1553	1557	rVV	264299	205514	5.51%	0.633%
14	11.469	1558	1561	1565	rVB	51714	47393	1.27%	0.146%
15	11.928	1635	1639	1642	rVB2	54387	70979	1.90%	0.219%
16	12.010	1650	1653	1655	rBV	68202	66769	1.79%	0.206%
17	12.610	1752	1755	1759	rBV	723752	598058	16.05%	1.841%
18	12.839	1788	1794	1798	rBV	635643	665726	17.86%	2.050%
19	12.980	1812	1818	1821	rBV	3298684	2963925	79.53%	9.125%
20	13.057	1827	1831	1835	rBV3	102624	112060	3.01%	0.345%
21	13.145	1842	1846	1847	rBV3	37427	47318	1.27%	0.146%
22	13.169	1847	1850	1852	rVB	76308	72159	1.94%	0.222%
23	13.233	1858	1861	1864	rBV	55852	45508	1.22%	0.140%
24	13.275	1864	1868	1870	rBV2	54712	63184	1.70%	0.195%
25	13.398	1886	1889	1892	rBV2	34010	39964	1.07%	0.123%
26	13.539	1910	1913	1917	rBV6	21768	39983	1.07%	0.123%
27	13.680	1934	1937	1942	rVB	65061	63426	1.70%	0.195%
28	13.745	1945	1948	1951	rVB	69079	54505	1.46%	0.168%
29	13.786	1951	1955	1958	rBV2	74382	86076	2.31%	0.265%
30	13.845	1962	1965	1966	rVV	54426	54566	1.46%	0.168%
31	13.886	1967	1972	1979	rVB3	133072	227858	6.11%	0.702%
32	14.039	1994	1998	2001	rBV2	1067649	1270272	34.08%	3.911%
33	14.069	2001	2003	2009	rVB	379072	321238	8.62%	0.989%
34	14.145	2014	2016	2019	rVB	64078	47101	1.26%	0.145%
35	14.269	2033	2037	2040	rVB2	40259	51187	1.37%	0.158%
36	14.427	2061	2064	2066	rVB	72668	61439	1.65%	0.189%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080322\
Data File : BF129550.D
Acq On : 03 Aug 2022 20:31
Operator : CG\JU
Sample : N3930-20
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-112

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-BF072522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.092	2172	2177	2180	rBV	410609	661054	17.74%	2.035%
38	15.198	2192	2195	2201	rVB	101758	130262	3.50%	0.401%
39	15.398	2225	2229	2235	rVB	254315	313532	8.41%	0.965%
40	15.463	2235	2240	2245	rVB	346147	416767	11.18%	1.283%
41	15.527	2246	2251	2254	rVV	731963	911190	24.45%	2.805%
42	15.557	2254	2256	2263	rVB	103573	131051	3.52%	0.403%
43	15.957	2321	2324	2331	rVB2	73902	116551	3.13%	0.359%
44	17.021	2500	2505	2518	rBV2	128171	324252	8.70%	0.998%
45	17.174	2523	2531	2542	rBV3	932959	2001690	53.71%	6.163%
46	17.510	2578	2588	2597	rBV	163963	550519	14.77%	1.695%
47	17.727	2620	2625	2637	rVB4	228188	538609	14.45%	1.658%
48	18.015	2669	2674	2682	rVB7	124661	305318	8.19%	0.940%

Sum of corrected areas: 32480391

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080322\
Data File : BF129550.D
Acq On : 03 Aug 2022 20:31
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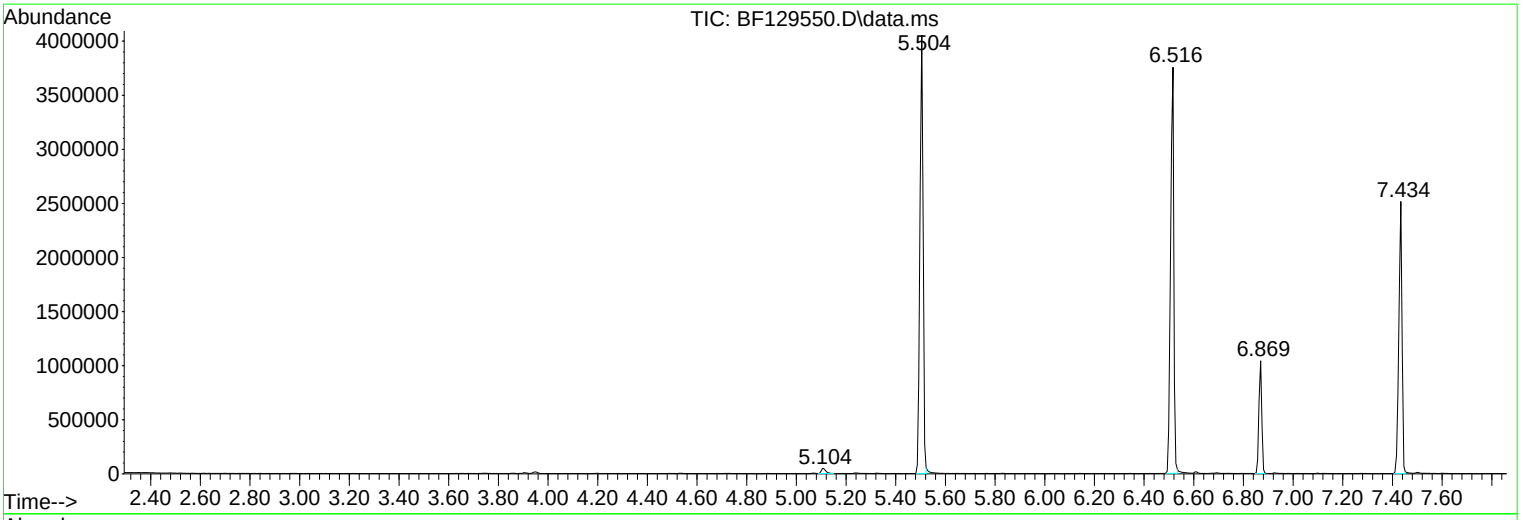
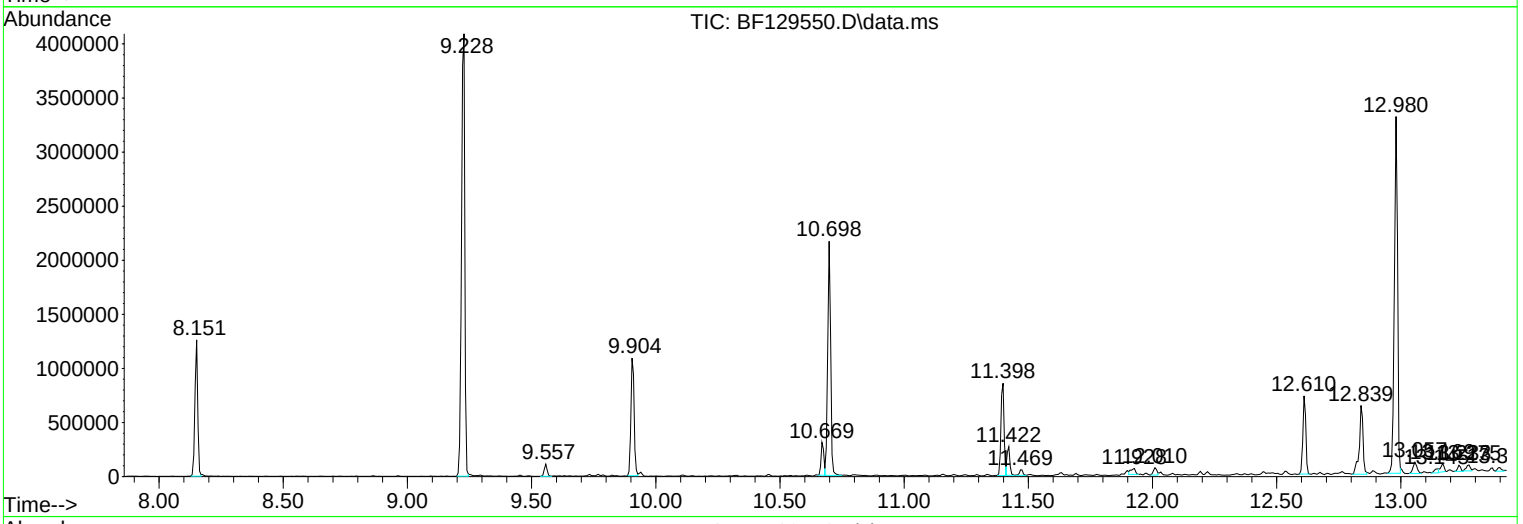
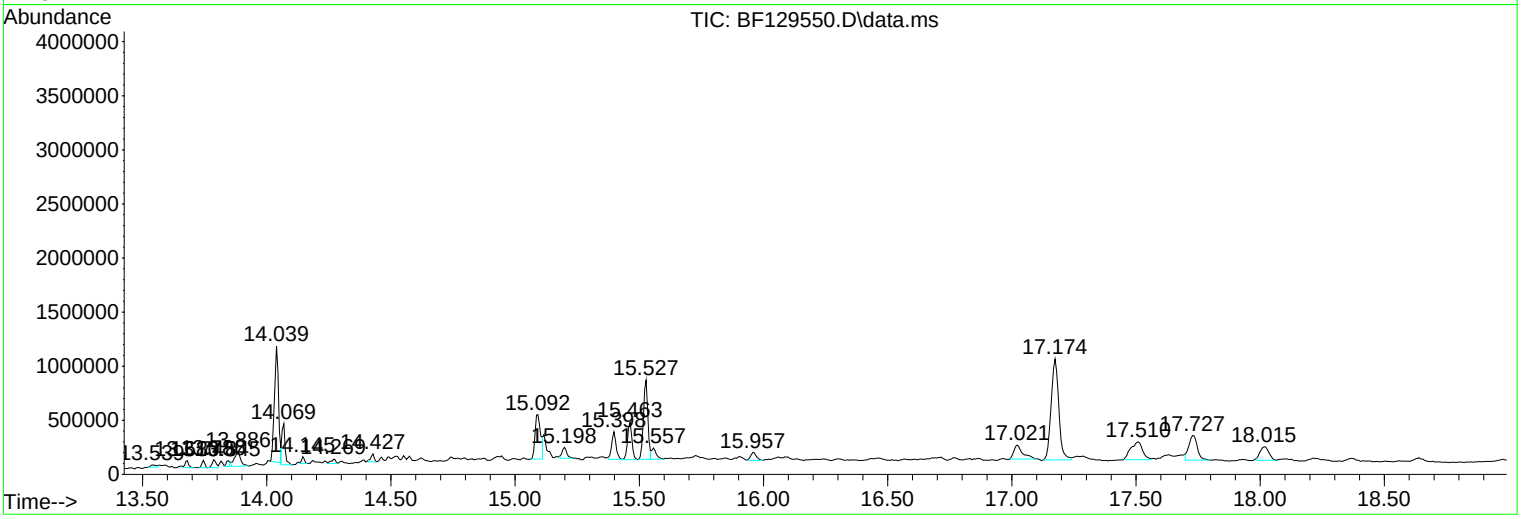
Instrument :
BNA_F
ClientSampleId :
RVE-112

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080322\
Data File : BF129550.D
Acq On : 03 Aug 2022 20:31
Operator : CG\JU
Sample : N3930-20
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

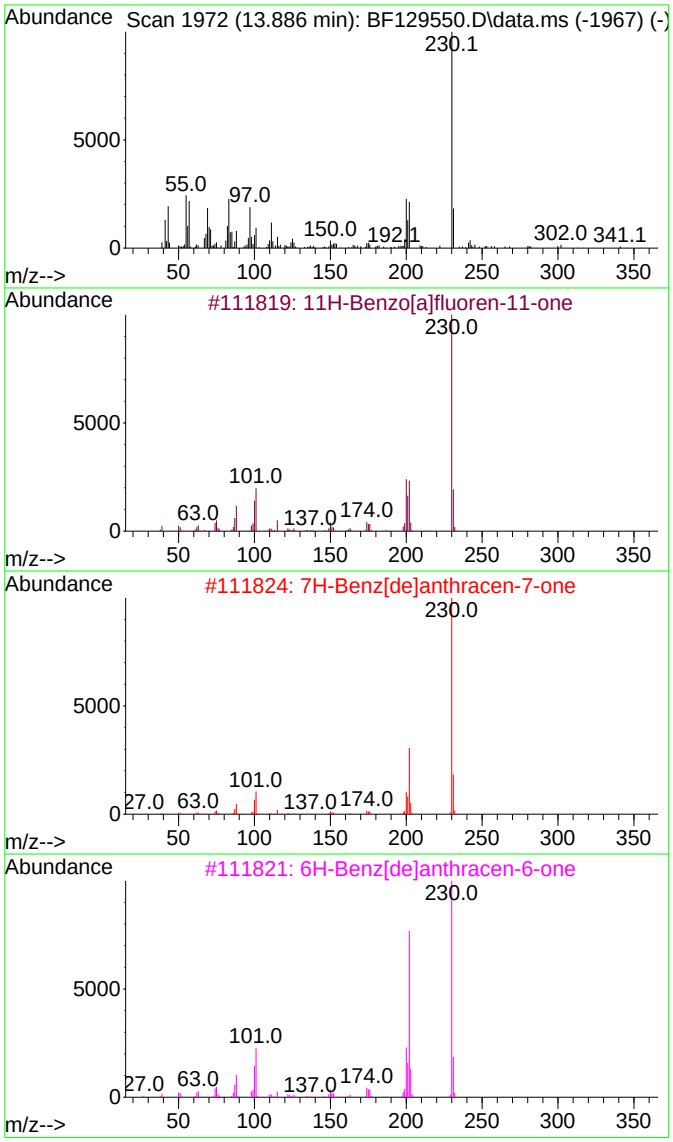
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

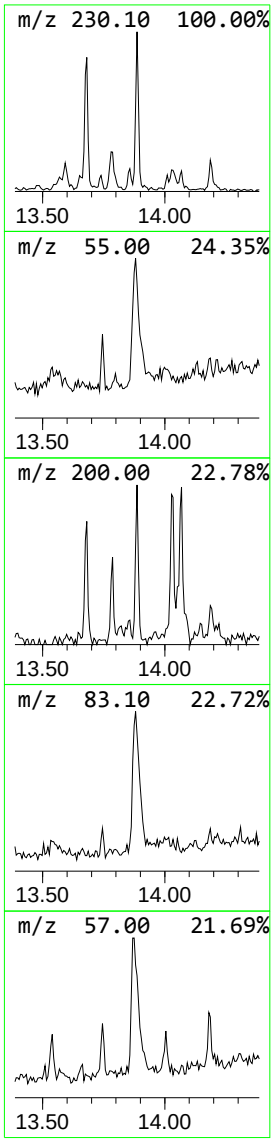
****

Peak Number 1 11H-Benzo[a]fluoren-11-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	3.59 ng	227858	Chrysene-d12	14.039

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	76
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	60
3	6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	49
4	benzonitrile, 2-(3-isoquinolinyl)-	230	C16H10N2	1000401-00-3	47
5	8-Hydroxyquinoline-5-carbaldehyd...	245	C13H15NO2Si	1010463-63-7	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080322\
Data File : BF129550.D
Acq On : 03 Aug 2022 20:31
Operator : CG\JU
Sample : N3930-20
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-112

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

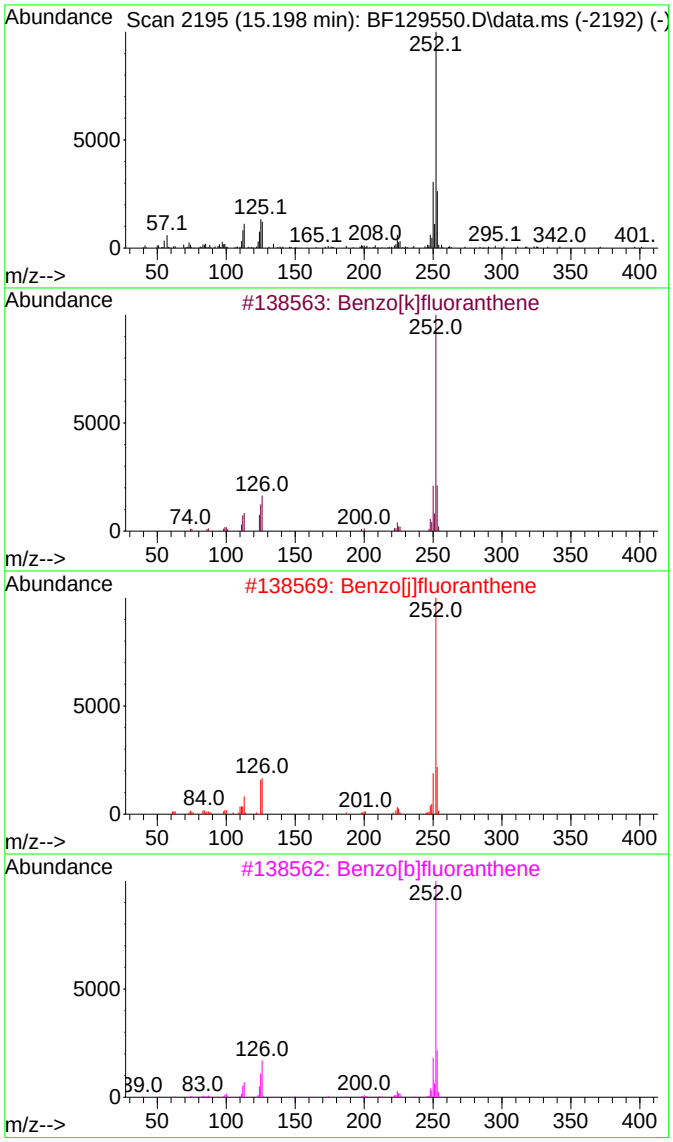
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

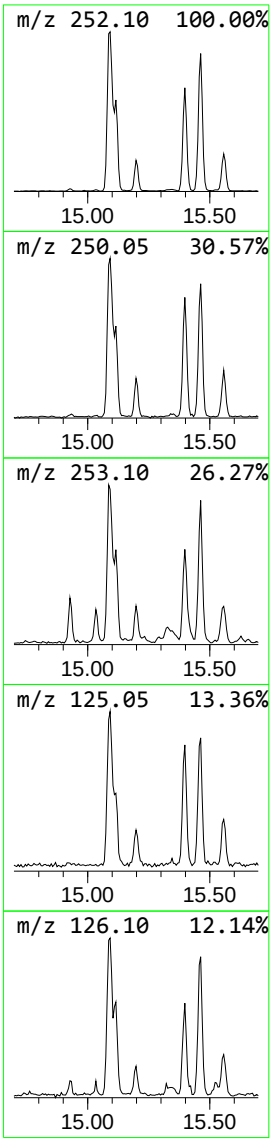
****

Peak Number 2 Benzo[j]fluoranthene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	2.86 ng	130262	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
2	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4	Benzo[e]pyrene	252	C20H12	000192-97-2	93
5	Benzo[a]pyrene	252	C20H12	000050-32-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080322\
Data File : BF129550.D
Acq On : 03 Aug 2022 20:31
Operator : CG\JU
Sample : N3930-20
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-112

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

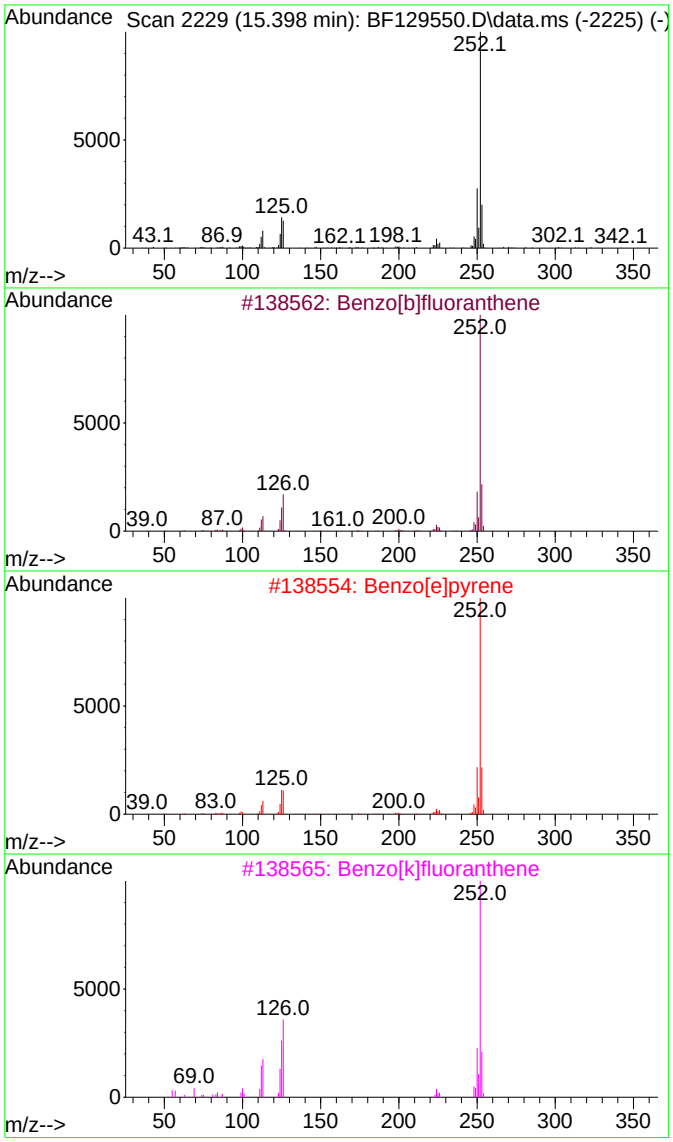
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

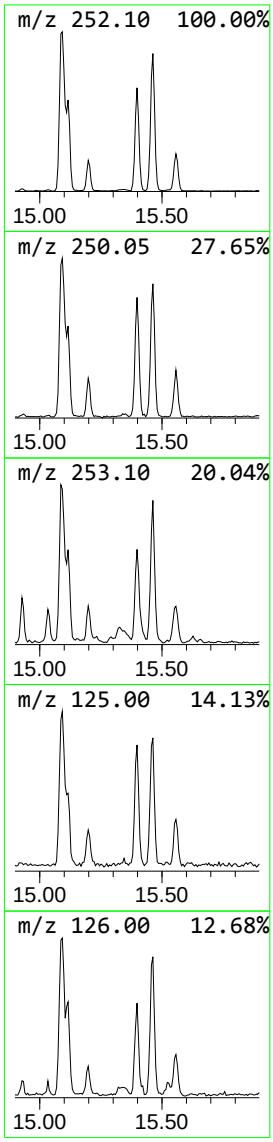
****

Peak Number 3 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	6.88 ng	313532	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
2	Benzo[e]pyrene	252	C20H12	000192-97-2	98
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	96
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
5	Benzo[a]pyrene	252	C20H12	000050-32-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080322\
Data File : BF129550.D
Acq On : 03 Aug 2022 20:31
Operator : CG\JU
Sample : N3930-20
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-112

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

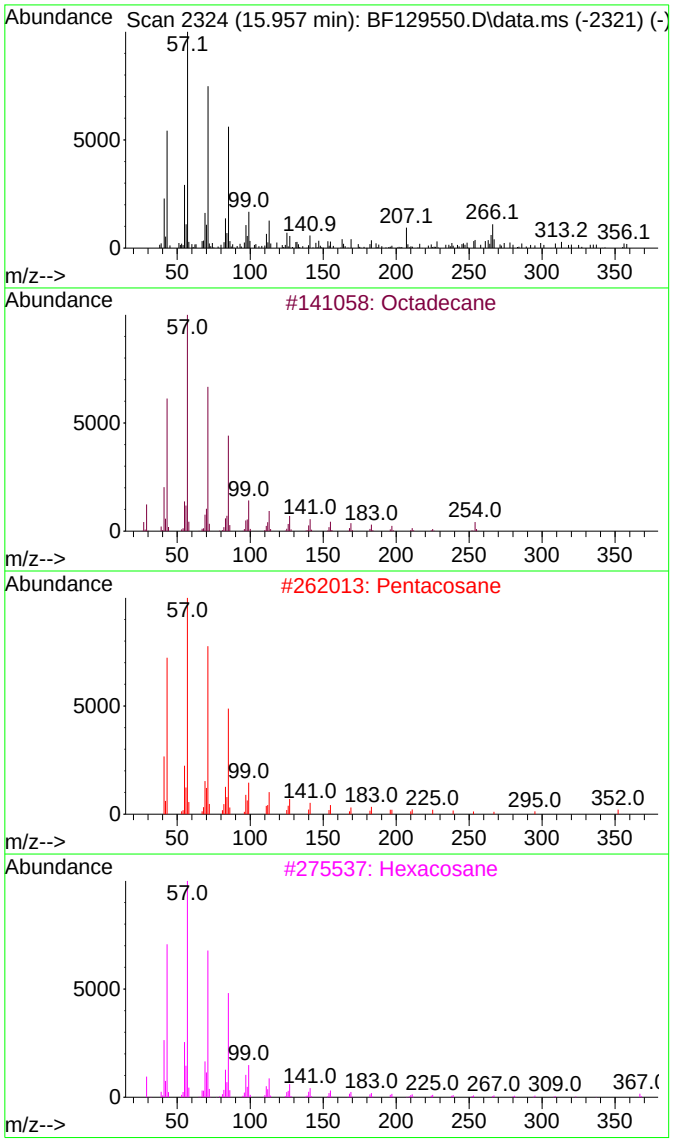
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

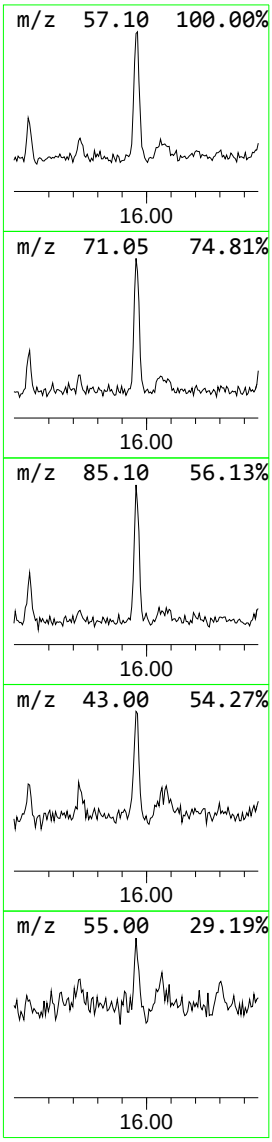
****

Peak Number 4 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.957	2.56 ng	116551	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	90
2	Pentacosane	352	C25H52	000629-99-2	74
3	Hexacosane	366	C26H54	000630-01-3	74
4	Octacosane	394	C28H58	000630-02-4	72
5	Heptacosane	380	C27H56	000593-49-7	72





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Data File : BF129550.D
Acq On : 03 Aug 2022 20:31
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Sample : N3930-20
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RVE-112

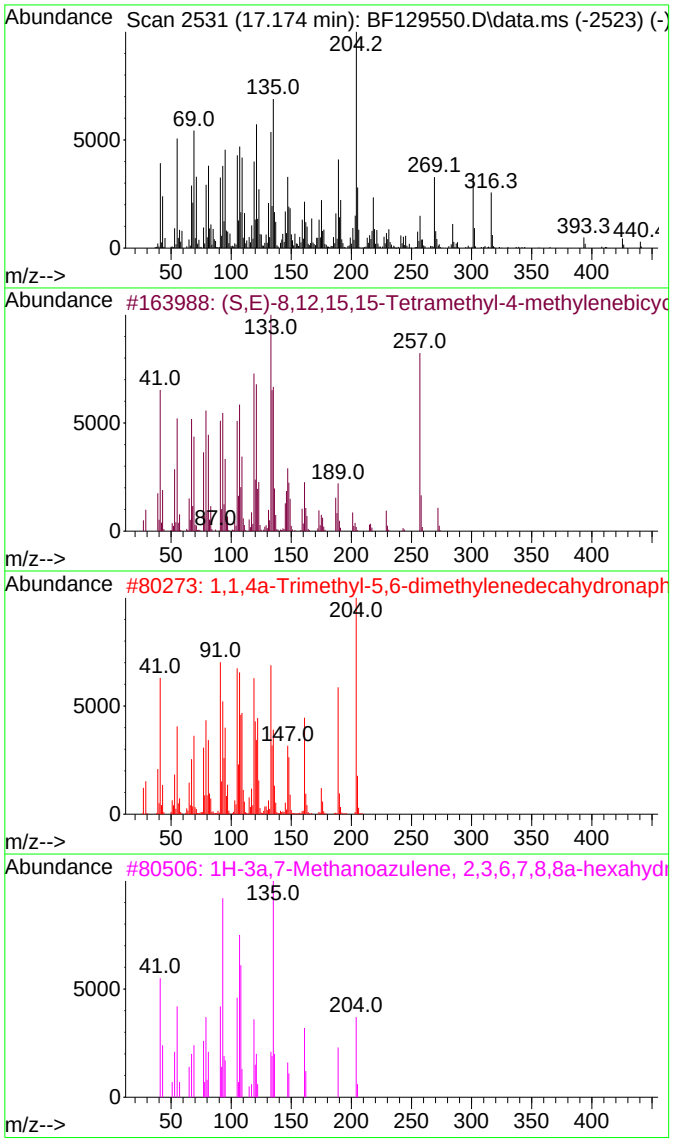
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

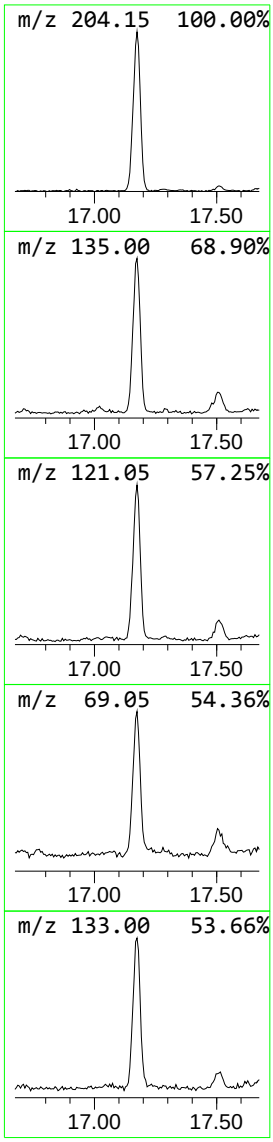
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (S,E)-8,12,15,15-Tetramethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.174	43.94 ng	2001690	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S,E)-8,12,15,15-Tetramethyl-4-m...	272	C20H32	386223-19-4	60
2	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	58
3	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	49
4	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	49
5	Farnesyl bromide	284	C15H25Br	006874-67-5	49





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Acq On : 03 Aug 2022 20:31
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Sample : N3930-20
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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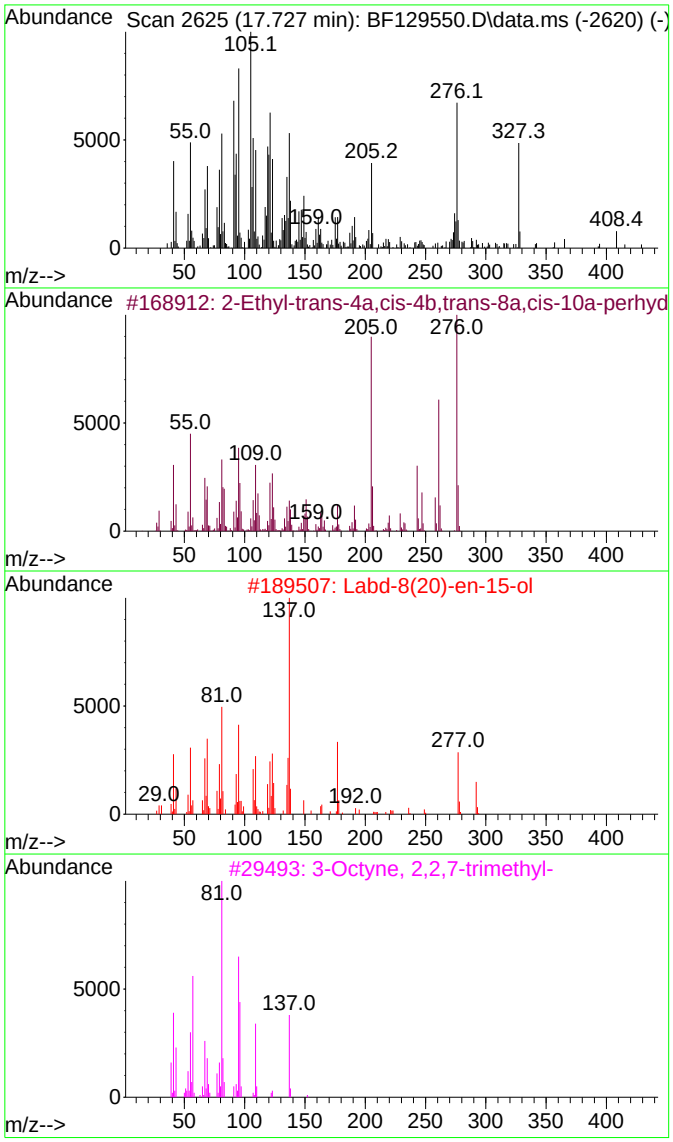
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

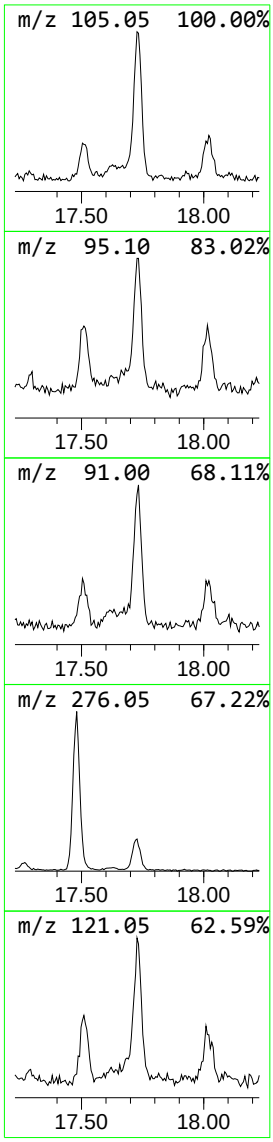
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Ethyl-trans-4a,cis-4b,tra... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.727	11.82 ng	538609	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethyl-trans-4a,cis-4b,trans-8a...	276	C19H32O	1000243-62-9	70
2	Labd-8(20)-en-15-ol	292	C20H36O	018318-72-4	25
3	3-Octyne, 2,2,7-trimethyl-	152	C11H20	055402-13-6	22
4	(E)-3-Methyl-5-((1R,4aR,8aR)-5,5...	290	C20H34O	021738-29-4	16
5	2-(p-Tolyl)oxazolo[4,5-c]quinoli...	276	C17H12N2O2	148563-22-8	15





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Acq On : 03 Aug 2022 20:31
Operator : CG\JU
Sample : N3930-20
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Instrument :
BNA_F
ClientSampleId :
RVE-112

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

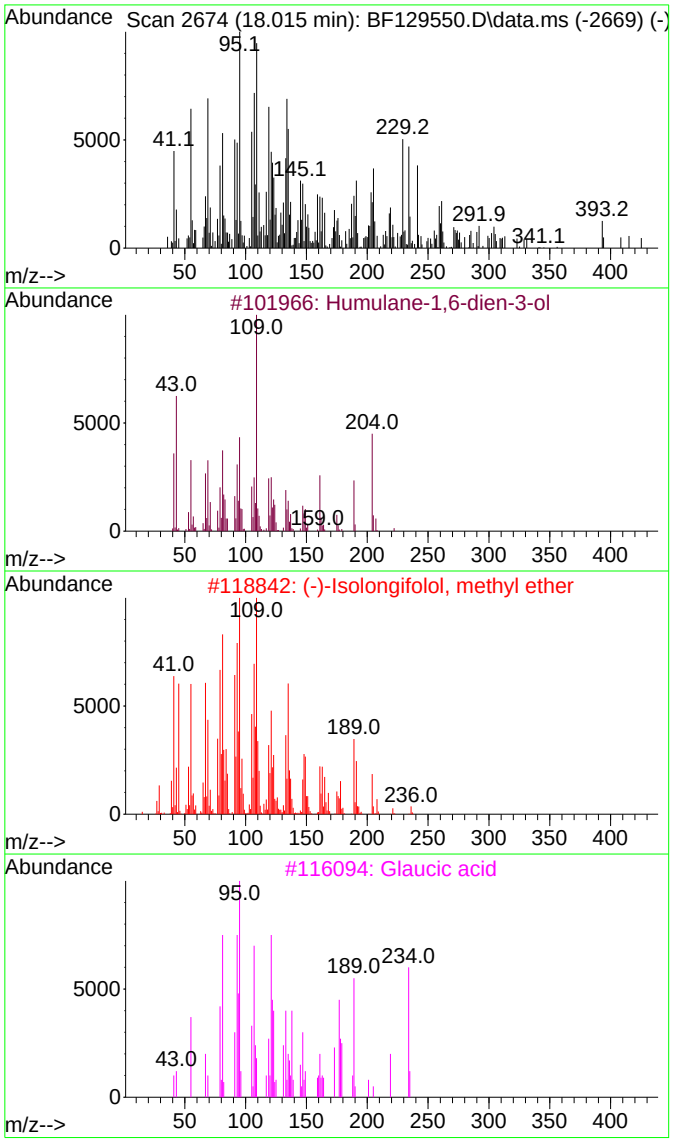
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

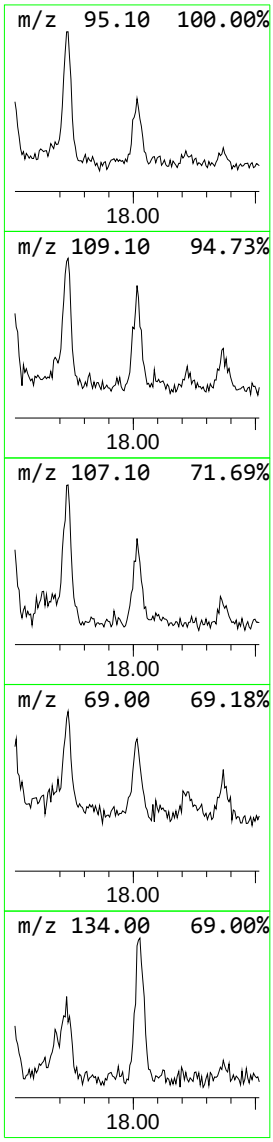
****

Peak Number 7 Humulane-1,6-dien-3-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.015	6.70 ng	305318	Perylene-d12	15.527

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Humulane-1,6-dien-3-ol	222	C15H26O	1000140-23-1	55
2	(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	47
3	Glaucic acid	234	C15H22O2	087745-30-0	38
4	Furan-2-carboxamide, N-ethyl-N-(...	229	C14H15NO2	1000308-20-3	38
5	p-Camphorene	272	C20H32	020016-72-2	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080322\
Data File : BF129550.D
Acq On : 03 Aug 2022 20:31
Operator : CG\JU
Sample : N3930-20
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072522.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
11H-Benzo[a]flu...	13.886	3.6	ng	227858	5	14.039	1270270	20.0
Benzo[j]fluoran...	15.198	2.9	ng	130262	6	15.527	911190	20.0
Benzo[e]pyrene	15.398	6.9	ng	313532	6	15.527	911190	20.0
Octadecane	15.957	2.6	ng	116551	6	15.527	911190	20.0
(S,E)-8,12,15,1...	17.174	43.9	ng	2001690	6	15.527	911190	20.0
2-Ethyl-trans-4...	17.727	11.8	ng	538609	6	15.527	911190	20.0
Humulane-1,6-di...	18.015	6.7	ng	305318	6	15.527	911190	20.0