LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121823\
Data File : BF136626.D
Acq On : 18 Dec 2023 21:17
Operator : CG\JU
Sample : 05485-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-14-STOCKPILE-BIN-5

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-BF120523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136626.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	15	19	27	rBV	24372	32351	1.33%	0.203%
2	5.028	495	500	508	rVB	232829	286943	11.77%	1.799%
3	5.434	565	569	573	rBV	2026461	1921381	78.82%	12.045%
4	6.434	735	739	742	rBV	1808637	1774908	72.81%	11.127%
5	6.786	796	799	803	rBV	509995	396589	16.27%	2.486%
6	7.351	890	895	898	rBV	1224828	1108455	45.47%	6.949%
7	8.063	1010	1016	1020	rBV	534952	442768	18.16%	2.776%
8	8.780	1134	1138	1142	rVB	42908	32842	1.35%	0.206%
9	8.875	1149	1154	1159	rVB	33917	31711	1.30%	0.199%
10	9.145	1195	1200	1203	rBV	2299890	1901681	78.01%	11.922%
11	9.410	1240	1245	1248	rBV	33071	37375	1.53%	0.234%
12	9.480	1254	1257	1259	rBV	45313	40412	1.66%	0.253%
13	9.680	1288	1291	1295	rBV	34592	28622	1.17%	0.179%
14	9.822	1309	1315	1319	rBV	547069	429948	17.64%	2.695%
15	10.369	1405	1408	1415	rVB2	36781	39174	1.61%	0.246%
16	10.616	1446	1450	1462	rVB	1360939	1130086	46.36%	7.085%
17	10.739	1466	1471	1478	rVB3	18926	28258	1.16%	0.177%
18	11.210	1549	1551	1556	rVB	37440	33620	1.38%	0.211%
19	11.316	1565	1569	1571	rBV	585250	480257	19.70%	3.011%
20	11.339	1571	1573	1576	rVV	218998	162999	6.69%	1.022%
21	11.392	1579	1582	1584	rVB	42147	39037	1.60%	0.245%
22	11.733	1633	1640	1643	rVB2	18488	30519	1.25%	0.191%
23	11.821	1651	1655	1657	rBV	65136	65077	2.67%	0.408%
24	11.851	1657	1660	1665	rVV	178042	178338	7.32%	1.118%
25	11.927	1670	1673	1676	rVV2	83261	100943	4.14%	0.633%
26	11.951	1676	1677	1681	rVB	52119	38703	1.59%	0.243%
27	12.116	1700	1705	1707	rBV2	34373	31754	1.30%	0.199%
28	12.374	1745	1749	1751	rBV	54491	57435	2.36%	0.360%
29	12.410	1751	1755	1757	rVV3	45205	54260	2.23%	0.340%
30	12.457	1760	1763	1767	rBV3	28498	37776	1.55%	0.237%
31	12.533	1772	1776	1780	rBV	339050	277716	11.39%	1.741%
32	12.639	1790	1794	1800	rBV6	54507	69878	2.87%	0.438%
33	12.763	1809	1815	1818	rBV	360902	352516	14.46%	2.210%
34	12.915	1836	1841	1844	rBV	2715478	2437754	100.00%	15.283%
35	12.986	1849	1853	1856	rBV3	33010	44087	1.81%	0.276%
36	13.068	1865	1867	1869	rBV3	29171	33535	1.38%	0.210%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121823\
Data File : BF136626.D
Acq On : 18 Dec 2023 21:17
Operator : CG\JU
Sample : 05485-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-14-STOCKPILE-BIN-5

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-BF120523.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.092	1869	1871	1875	rVB2	68850	68592	2.81%	0.430%
38	13.162	1881	1883	1886	rVB	49771	38695	1.59%	0.243%
39	13.198	1886	1889	1892	rBV2	61845	62682	2.57%	0.393%
40	13.292	1902	1905	1907	rVB	38420	29969	1.23%	0.188%
41	13.321	1907	1910	1913	rBV	41542	41073	1.68%	0.257%
42	13.821	1992	1995	1998	rVB2	45080	41285	1.69%	0.259%
43	13.968	2015	2020	2023	rBV2	632143	712695	29.24%	4.468%
44	13.992	2023	2024	2028	rVB	146167	114035	4.68%	0.715%
45	14.139	2047	2049	2055	rVB4	39293	45491	1.87%	0.285%
46	15.015	2195	2198	2201	rBV	112122	153418	6.29%	0.962%
47	15.386	2258	2261	2267	rVB	97898	117364	4.81%	0.736%
48	15.451	2268	2272	2276	rBV	268901	336029	13.78%	2.107%

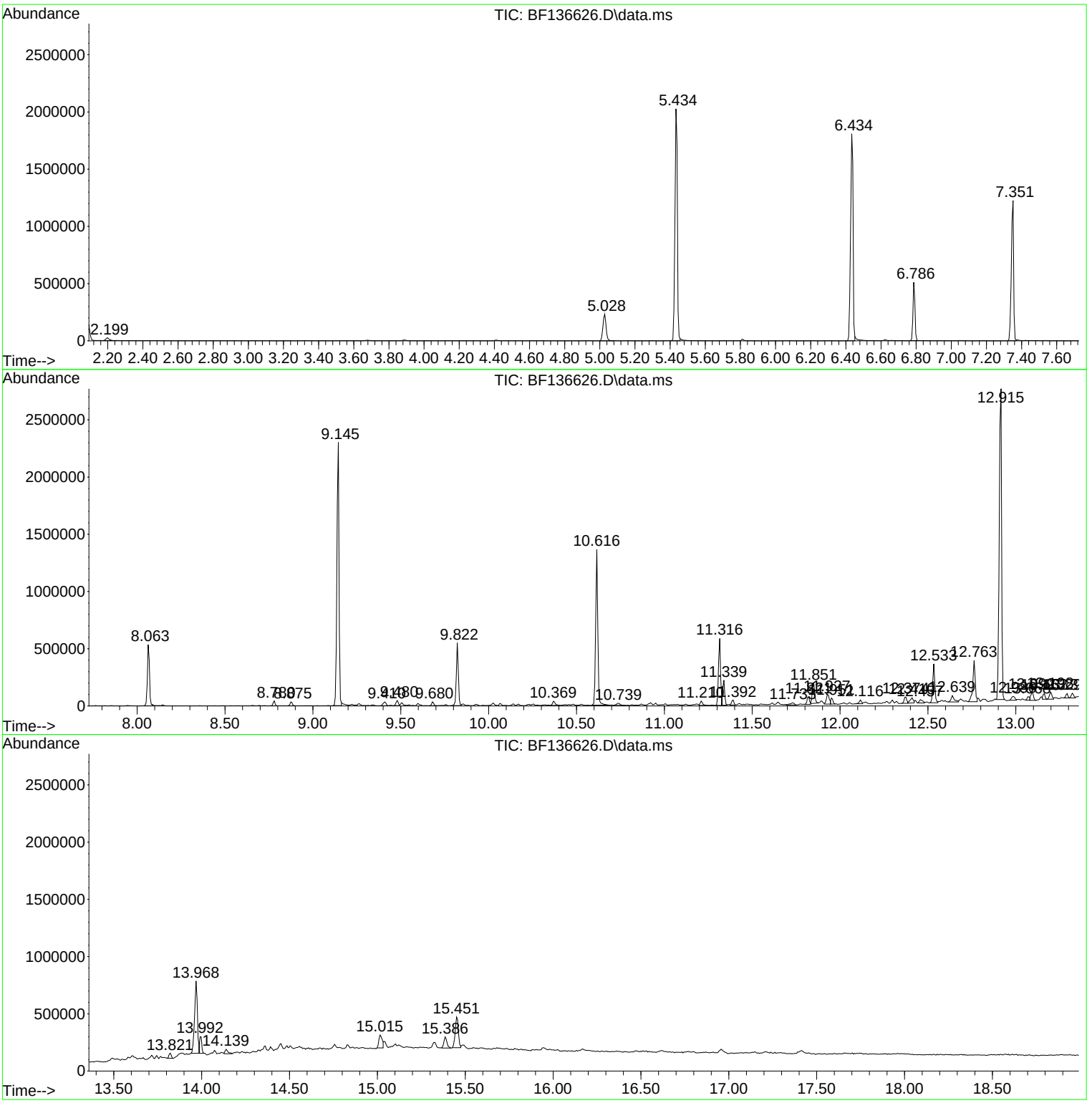
Sum of corrected areas: 15951036

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121823\
Data File : BF136626.D
Acq On : 18 Dec 2023 21:17
Operator : CG\JU
Sample : 05485-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-14-STOCKPILE-BIN-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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\BF121823\
Data File : BF136626.D
Acq On : 18 Dec 2023 21:17
Operator : CG\JU
Sample : 05485-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-14-STOCKPILE-BIN-5

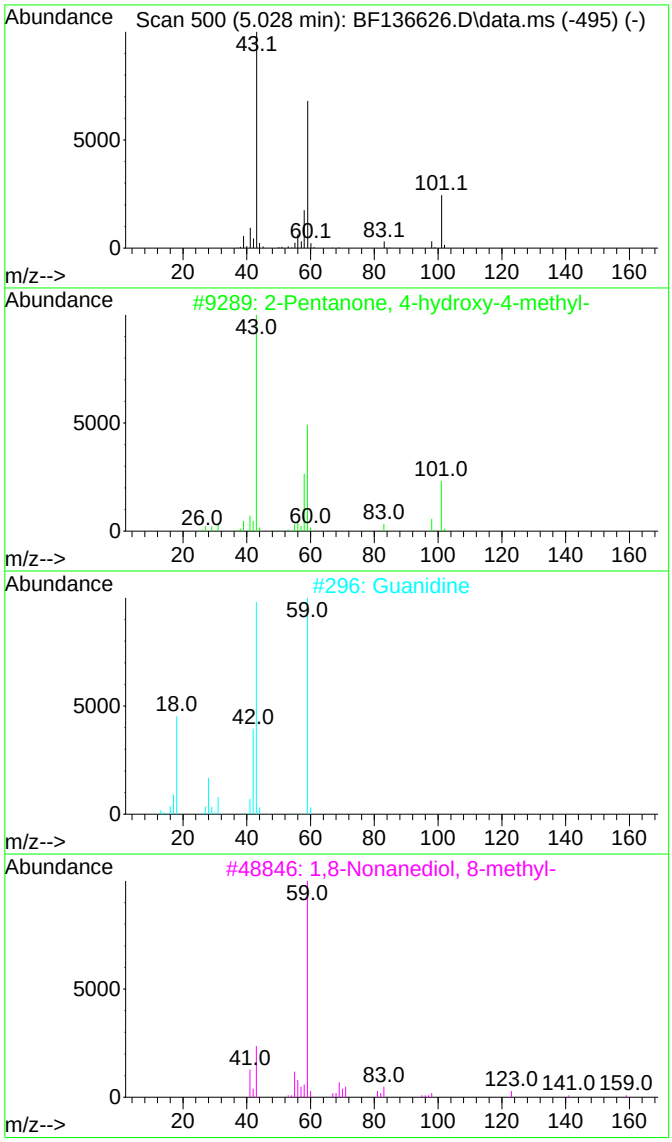
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

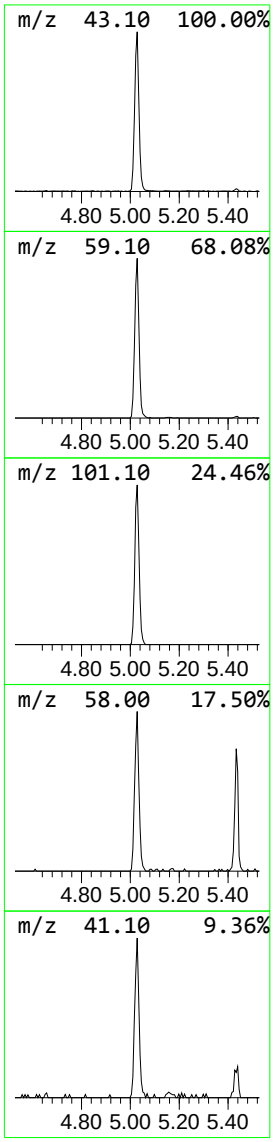
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	14.47 ng	286943	1,4-Dichlorobenzene-d4	6.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Guanidine	59	CH5N3	000113-00-8	43
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121823\
Data File : BF136626.D
Acq On : 18 Dec 2023 21:17
Operator : CG\JU
Sample : 05485-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-14-STOCKPILE-BIN-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

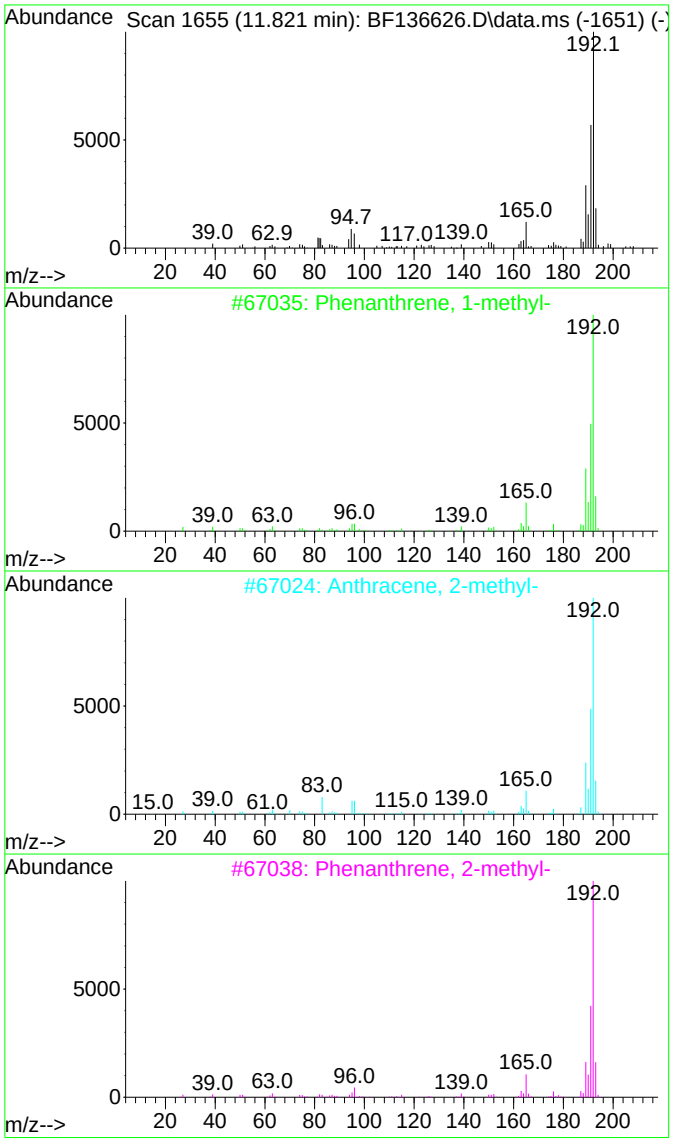
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

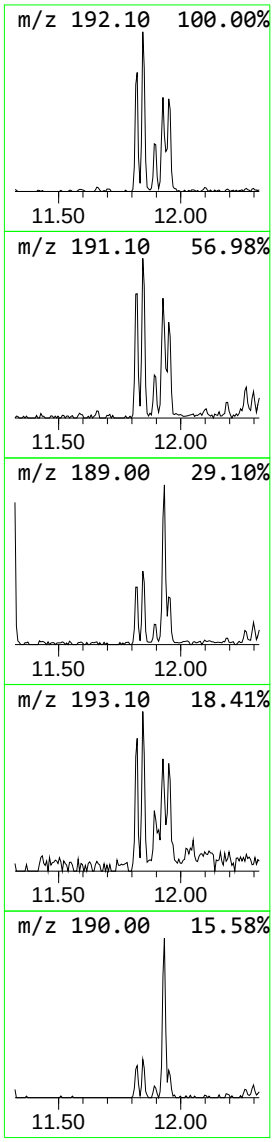
****

Peak Number 2 Phenanthrene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.821	2.71 ng	65077	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	95
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
5	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121823\
Data File : BF136626.D
Acq On : 18 Dec 2023 21:17
Operator : CG\JU
Sample : 05485-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-14-STOCKPILE-BIN-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

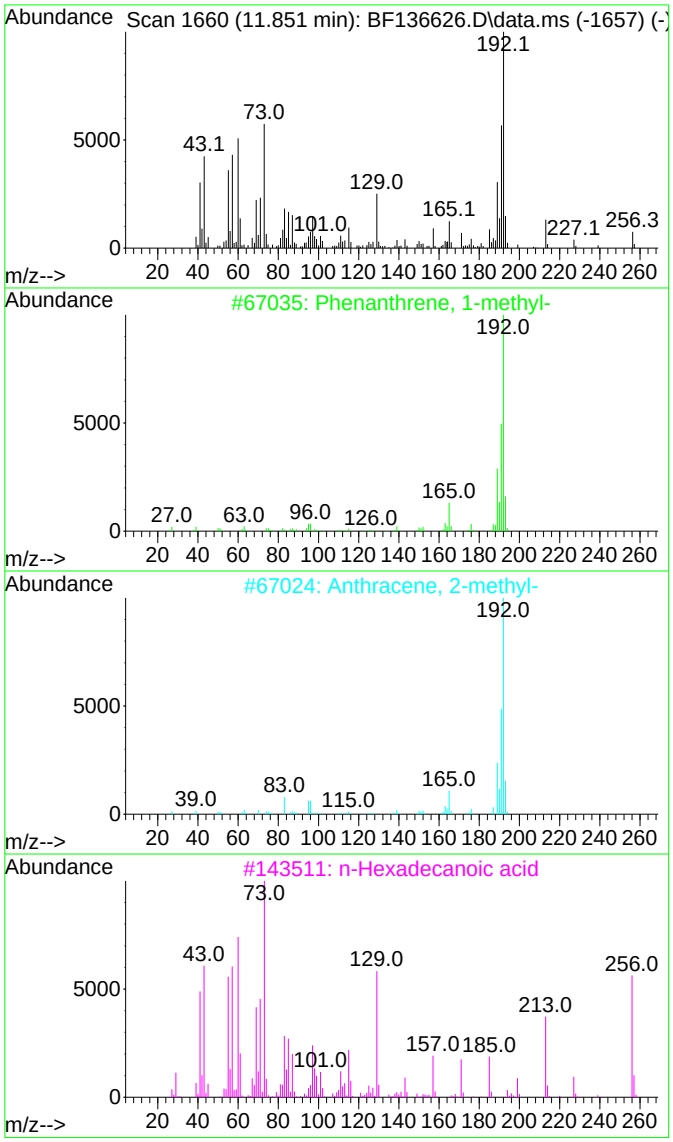
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

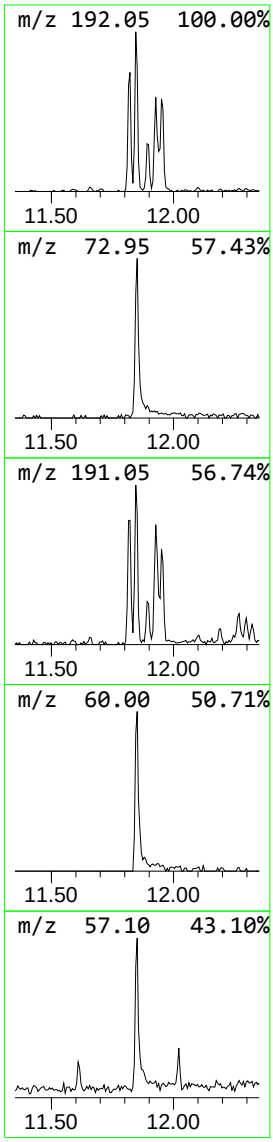
****

Peak Number 3 Anthracene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	7.43 ng	178338	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	92
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	92
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	91
5	1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121823\
Data File : BF136626.D
Acq On : 18 Dec 2023 21:17
Operator : CG\JU
Sample : 05485-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-14-STOCKPILE-BIN-5

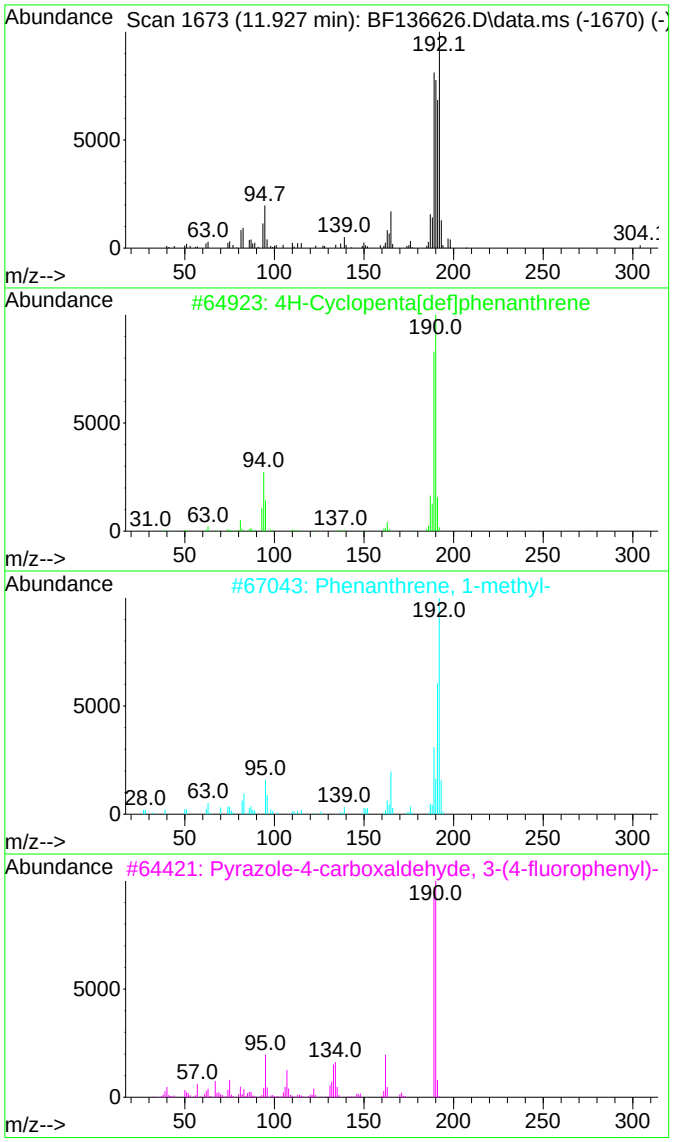
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

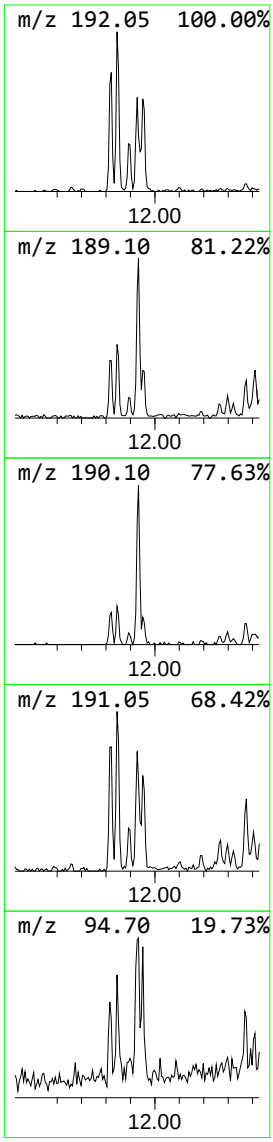
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	4.20 ng	100943	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	55
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	46
3	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	43
4	Naphtho[1,2-b]norbornadiene	192	C15H12	1000210-14-8	42
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121823\
Data File : BF136626.D
Acq On : 18 Dec 2023 21:17
Operator : CG\JU
Sample : 05485-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-14-STOCKPILE-BIN-5

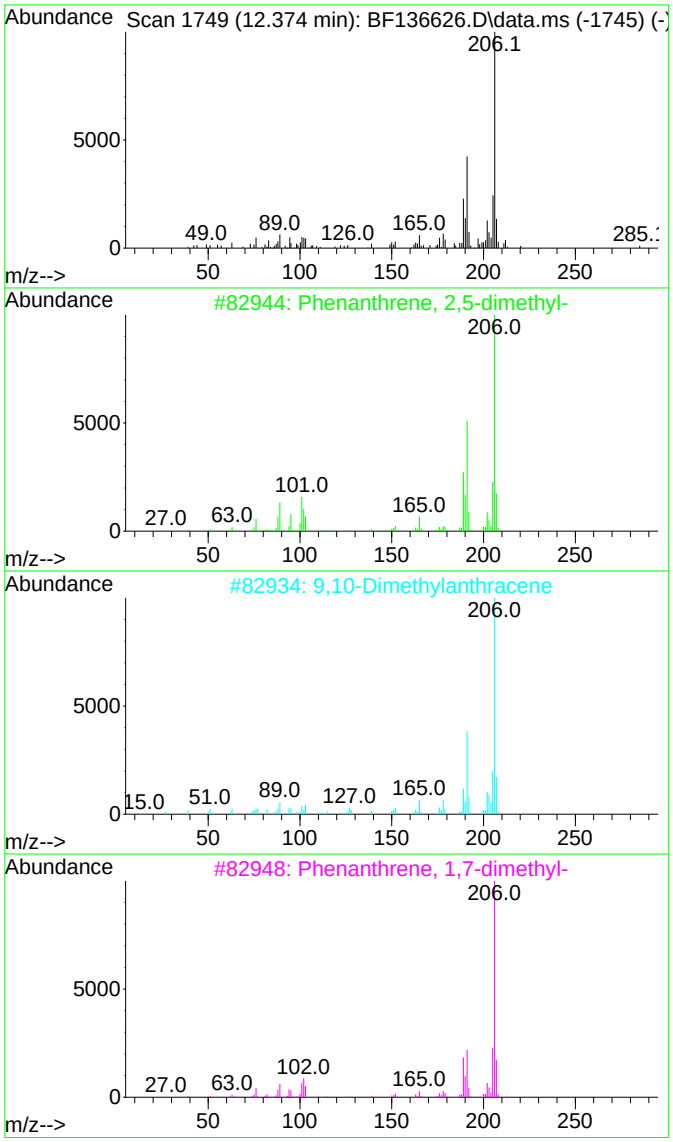
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

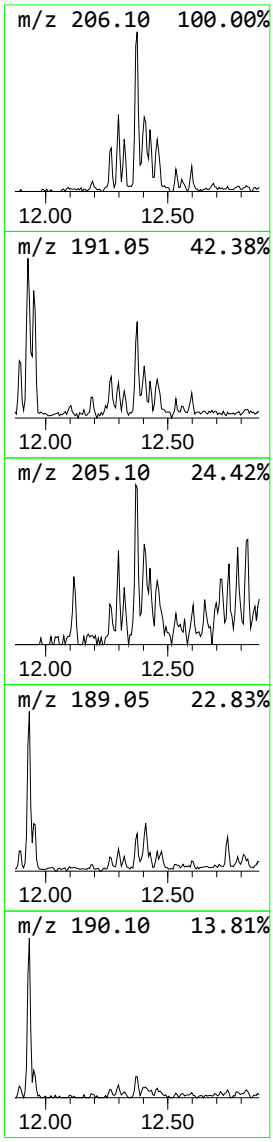
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phenanthrene, 2,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.374	2.39 ng	57435	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	93
3	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	89
4	di-p-Tolylacetylene	206	C16H14	002789-88-0	87
5	Phenanthrene, 2,7-dimethyl-	206	C16H14	001576-69-8	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121823\
Data File : BF136626.D
Acq On : 18 Dec 2023 21:17
Operator : CG\JU
Sample : 05485-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-14-STOCKPILE-BIN-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

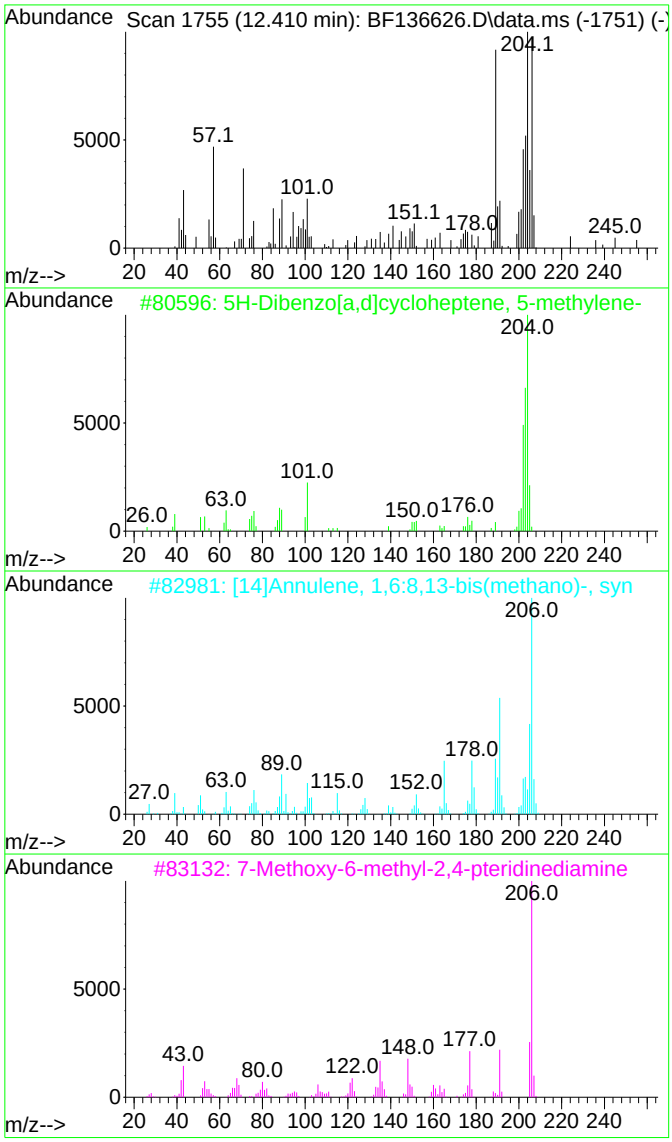
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

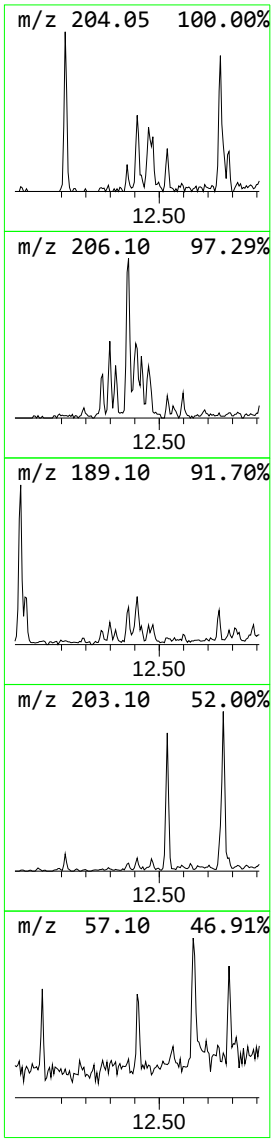
****

Peak Number 6 unknown12.410 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.410	2.26 ng	54260	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Dibenzo[a,d]cycloheptene, 5-m...	204	C16H12	002975-79-3	38
2	[14]Annulene, 1,6:8,13-bis(metha...	206	C16H14	085385-68-8	30
3	7-Methoxy-6-methyl-2,4-pteridine...	206	C8H10N6O	343347-40-0	25
4	Naphthalene, 1-phenyl-	204	C16H12	000605-02-7	25
5	Isoquinoline, 1,2,3,4-tetrahydro...	205	C12H19NSi	069944-96-3	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121823\
Data File : BF136626.D
Acq On : 18 Dec 2023 21:17
Operator : CG\JU
Sample : 05485-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-14-STOCKPILE-BIN-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

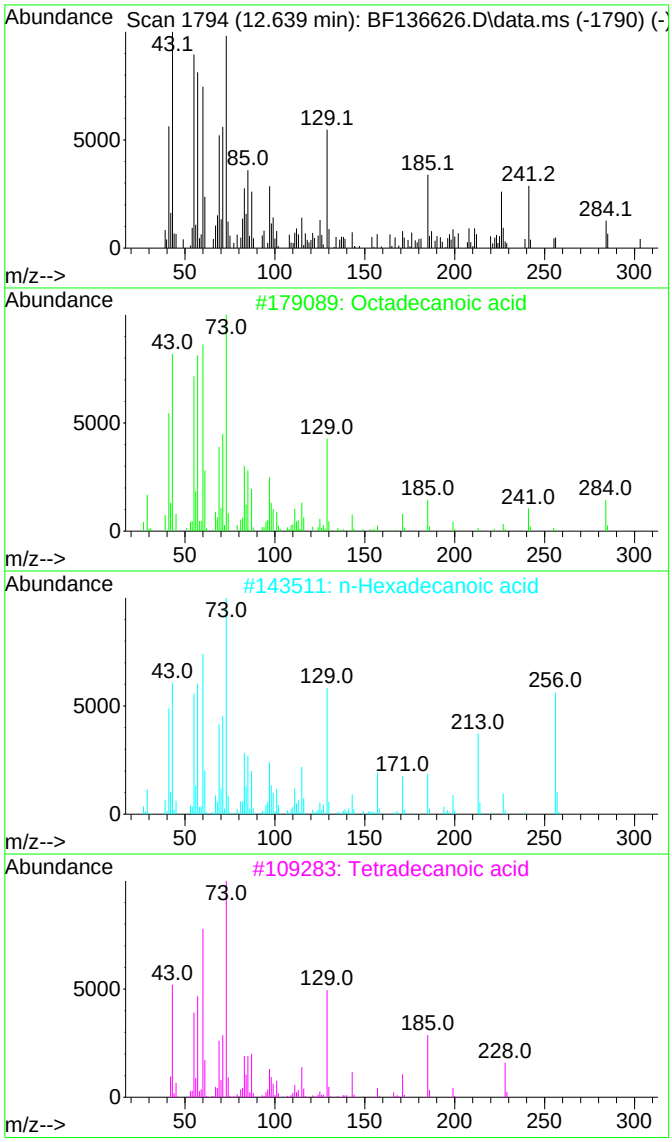
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

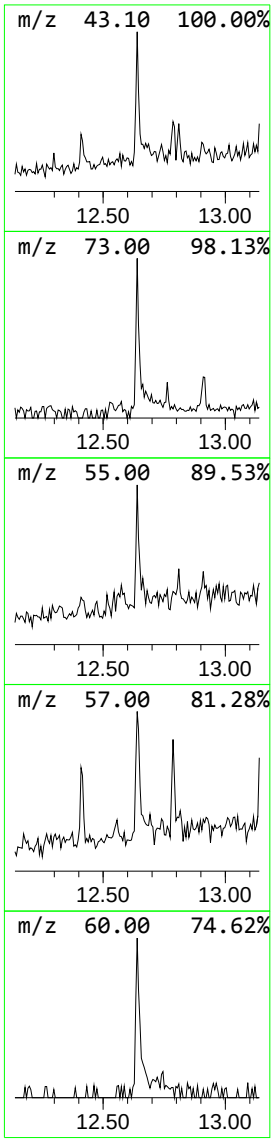
****

Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.639	2.91 ng	69878	Phenanthrene-d10	11.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	90
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4	n-Decanoic acid	172	C10H20O2	000334-48-5	50
5	Silane, methylvinyl(cycloheptylo...	242	C13H26O2Si	1000421-02-6	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121823\
Data File : BF136626.D
Acq On : 18 Dec 2023 21:17
Operator : CG\JU
Sample : 05485-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-14-STOCKPILE-BIN-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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
2-Pentanone, 4-...	5.028	14.5	ng	286943	1	6.786	396589	20.0
Phenanthrene, 1...	11.821	2.7	ng	65077	4	11.316	480257	20.0
Anthracene, 2-m...	11.851	7.4	ng	178338	4	11.316	480257	20.0
4H-Cyclopenta[d...	11.927	4.2	ng	100943	4	11.316	480257	20.0
Phenanthrene, 2...	12.374	2.4	ng	57435	4	11.316	480257	20.0
unknown12.410	12.410	2.3	ng	54260	4	11.316	480257	20.0
Octadecanoic acid	12.639	2.9	ng	69878	4	11.316	480257	20.0