LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110724\
Data File : BF140278.D
Acq On : 07 Nov 2024 16:39
Operator : RC/JU
Sample : P4694-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Z-04

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-BF110524.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF140278.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	7	14	27	rVB	1119539	1838445	52.30%	5.264%
2	2.287	28	33	46	rVB	41711	75760	2.16%	0.217%
3	5.104	501	512	524	rVB	104346	165098	4.70%	0.473%
4	5.498	572	579	584	rBV	2281655	3089517	87.88%	8.847%
5	6.498	742	749	754	rBV	2331912	3227212	91.80%	9.241%
6	6.875	808	813	819	rVB	608973	757171	21.54%	2.168%
7	7.269	876	880	884	rBV2	26248	40343	1.15%	0.116%
8	7.434	898	908	913	rBV	1561942	2116813	60.21%	6.062%
9	7.516	918	922	926	rVB4	25833	37528	1.07%	0.107%
10	7.687	947	951	956	rVB2	47884	65776	1.87%	0.188%
11	8.157	1025	1031	1038	rBV	752577	990646	28.18%	2.837%
12	8.369	1063	1067	1075	rBV2	22705	39516	1.12%	0.113%
13	9.234	1208	1214	1219	rBV	2800860	3515427	100.00%	10.067%
14	9.310	1223	1227	1235	rVV3	25055	40689	1.16%	0.117%
15	9.569	1266	1271	1274	rBV	26918	39348	1.12%	0.113%
16	9.916	1322	1330	1333	rBV	798781	1047388	29.79%	2.999%
17	9.945	1333	1335	1339	rVB	82444	87233	2.48%	0.250%
18	10.116	1360	1364	1368	rBV	52020	66864	1.90%	0.191%
19	10.339	1394	1402	1409	rBV4	25396	50539	1.44%	0.145%
20	10.463	1418	1423	1428	rVB	83211	107009	3.04%	0.306%
21	10.628	1446	1451	1456	rVB	208263	268577	7.64%	0.769%
22	10.704	1458	1464	1476	rVV	1582638	2051884	58.37%	5.876%
23	10.822	1479	1484	1491	rVB4	31896	61826	1.76%	0.177%
24	11.010	1510	1516	1519	rBV4	28763	52292	1.49%	0.150%
25	11.210	1546	1550	1553	rVB	35073	45134	1.28%	0.129%
26	11.263	1553	1559	1562	rVV3	37121	64343	1.83%	0.184%
27	11.298	1562	1565	1571	rVB	51075	68664	1.95%	0.197%
28	11.404	1578	1583	1585	rBV	701143	955301	27.17%	2.736%
29	11.428	1585	1587	1591	rVV	775350	849180	24.16%	2.432%
30	11.475	1591	1595	1599	rVV	155082	228676	6.50%	0.655%
31	11.633	1616	1622	1629	rBV2	87772	155054	4.41%	0.444%
32	11.933	1669	1673	1678	rVB2	279373	381076	10.84%	1.091%
33	11.980	1678	1681	1684	rVV	36482	43551	1.24%	0.125%
34	12.022	1684	1688	1695	rVB2	163801	307494	8.75%	0.881%
35	12.104	1695	1702	1706	rBV5	24079	48760	1.39%	0.140%
36	12.198	1711	1718	1721	rBV2	65301	132479	3.77%	0.379%

LSC Area Percent Report

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Sample : P4694-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
Z-04

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-BF110524.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	12.351	1739	1744	1747	rBV3	38834	56527	1.61%	0.162%
38	12.457	1758	1762	1765	rBV	51966	68060	1.94%	0.195%
39	12.492	1765	1768	1773	rVV3	35782	51335	1.46%	0.147%
40	12.539	1773	1776	1782	rVB3	49491	75102	2.14%	0.215%
41	12.622	1784	1790	1794	rBV	967852	1253819	35.67%	3.590%
42	12.663	1794	1797	1803	rVB3	30351	50270	1.43%	0.144%
43	12.716	1803	1806	1809	rBV	44202	56625	1.61%	0.162%
44	12.851	1822	1829	1834	rBV	841794	1261960	35.90%	3.614%
45	12.898	1834	1837	1843	rVB2	48043	71892	2.05%	0.206%
46	12.992	1844	1853	1860	rBV	1992404	2635848	74.98%	7.548%
47	13.063	1860	1865	1870	rBV2	72355	140904	4.01%	0.403%
48	13.174	1877	1884	1888	rVB	119936	229750	6.54%	0.658%
49	13.245	1888	1896	1899	rBV2	85736	138348	3.94%	0.396%
50	13.280	1899	1902	1909	rVB2	98617	150728	4.29%	0.432%
51	13.374	1915	1918	1920	rBV2	41933	48118	1.37%	0.138%
52	13.404	1920	1923	1927	rVB3	47683	58419	1.66%	0.167%
53	13.569	1946	1951	1955	rBV6	37550	96961	2.76%	0.278%
54	13.686	1967	1971	1976	rVB	75687	104695	2.98%	0.300%
55	13.798	1985	1990	1992	rBV2	83986	129887	3.69%	0.372%
56	13.827	1992	1995	1997	rVV	34396	43614	1.24%	0.125%
57	13.898	2003	2007	2015	rVB2	131475	217765	6.19%	0.624%
58	14.045	2025	2032	2036	rBV2	895708	1668264	47.46%	4.777%
59	14.157	2048	2051	2054	rVB	54418	59364	1.69%	0.170%
60	14.433	2095	2098	2102	rVV	76389	94840	2.70%	0.272%
61	14.468	2102	2104	2108	rVB2	41668	48536	1.38%	0.139%
62	14.816	2160	2163	2169	rVB2	56176	97680	2.78%	0.280%
63	15.104	2206	2212	2220	rBV	396931	909922	25.88%	2.606%
64	15.210	2227	2230	2235	rVB	57235	72342	2.06%	0.207%
65	15.410	2259	2264	2270	rVB	194736	321816	9.15%	0.922%
66	15.474	2270	2275	2280	rVB	278264	421347	11.99%	1.207%
67	15.539	2280	2286	2298	rVB2	375499	720307	20.49%	2.063%
68	17.033	2535	2540	2551	rVB2	110504	252086	7.17%	0.722%
69	17.492	2612	2618	2630	rVB	81228	202023	5.75%	0.579%

Sum of corrected areas: 34921767

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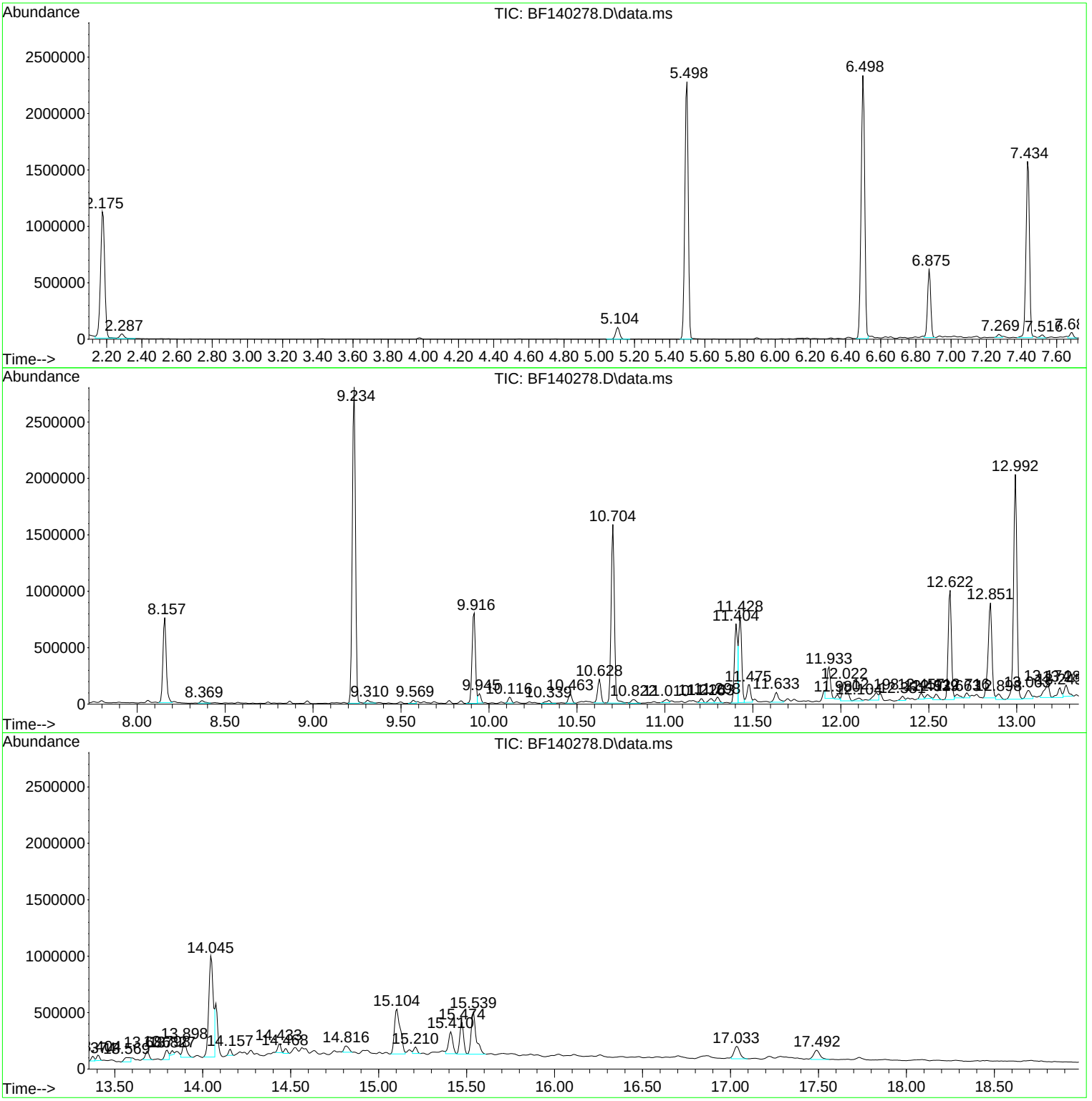
BNA_F
ClientSampleId :
Z-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.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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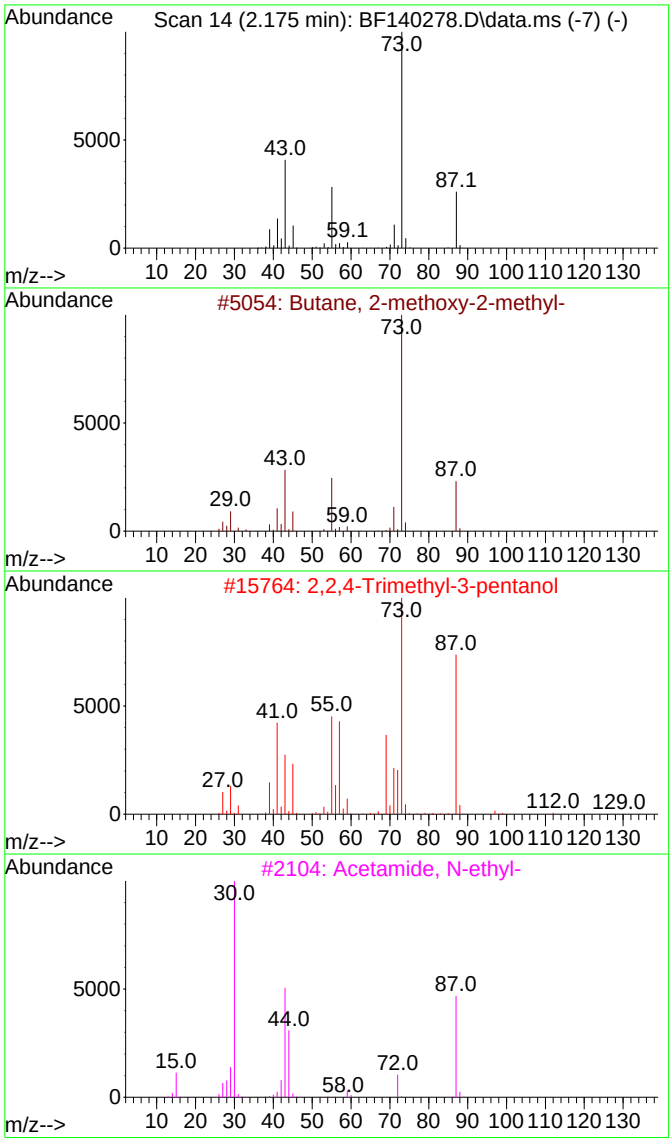
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

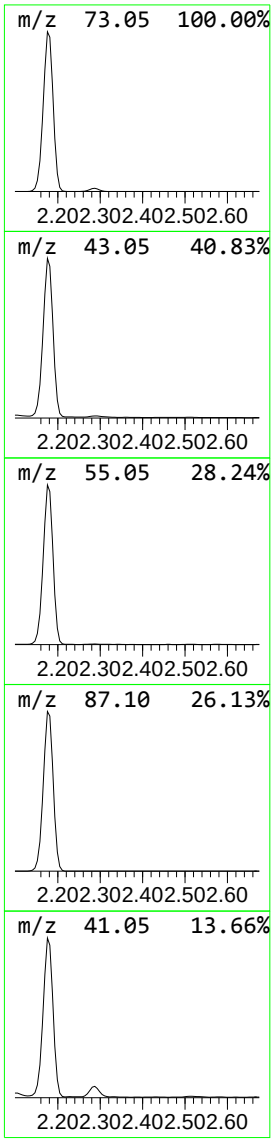
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	48.56 ng	1838450	1,4-Dichlorobenzene-d4	6.875

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	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17





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Data File : BF140278.D
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Sample : P4694-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Z-04

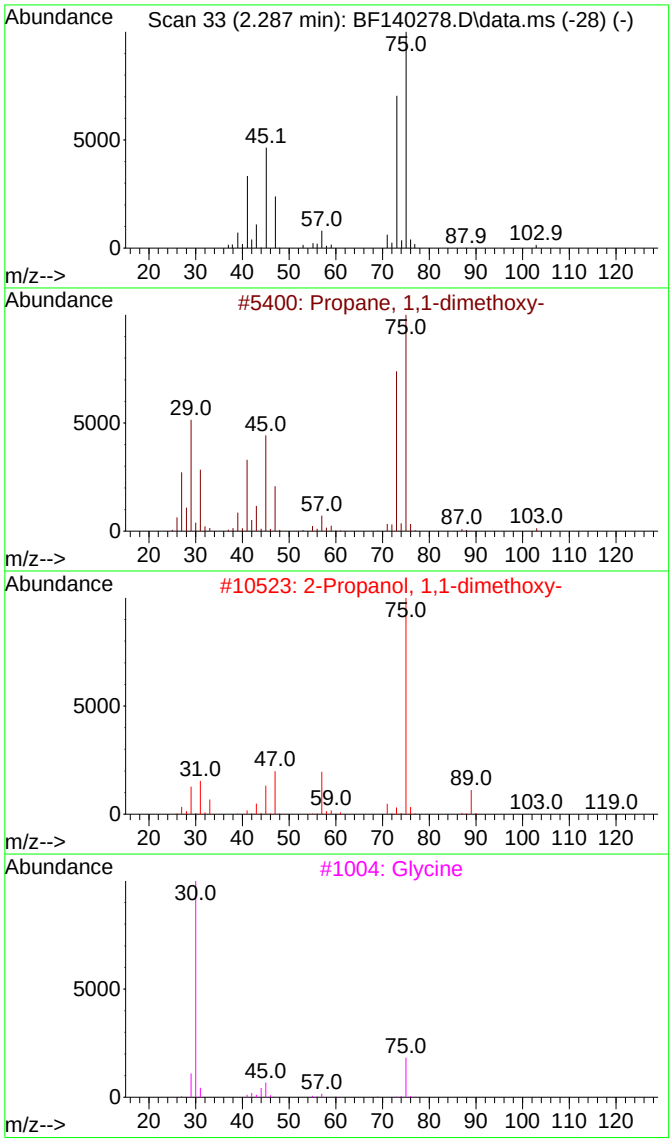
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

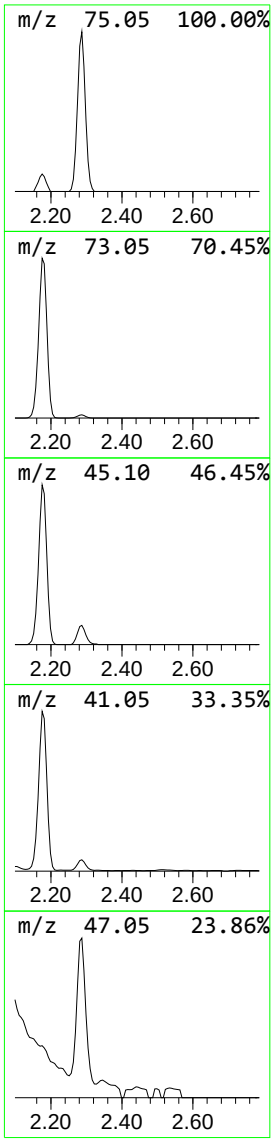
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	2.00 ng	75760	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	56
2	2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	36
3	Glycine	75	C2H5NO2	000056-40-6	9
4	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
5	Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	9





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Sample : P4694-05
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Instrument :
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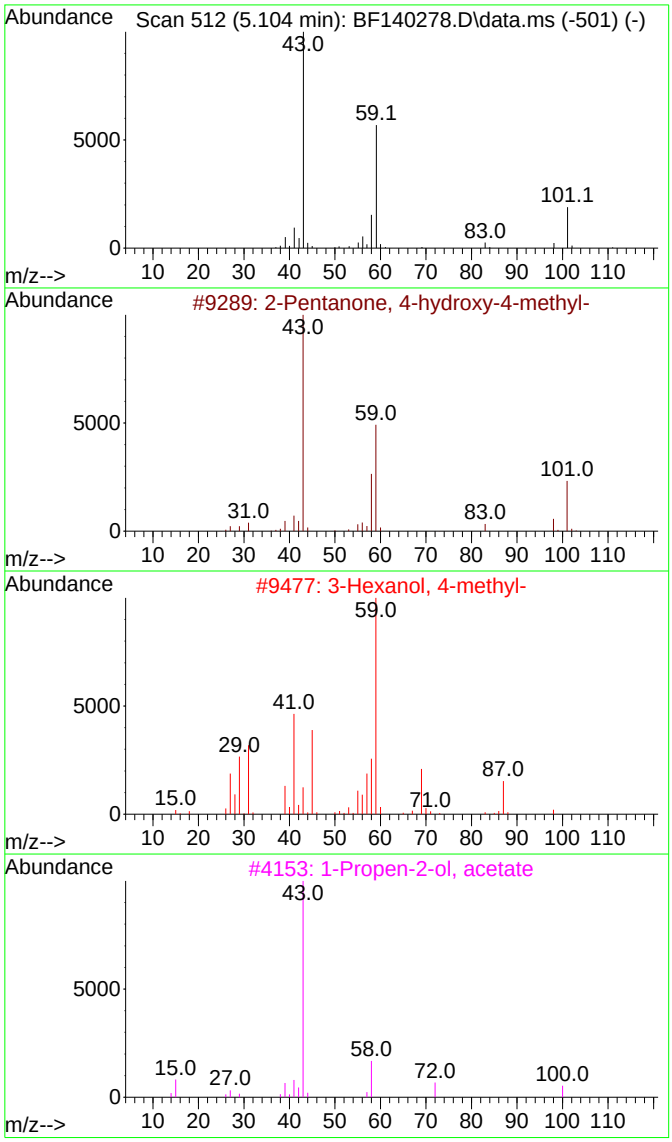
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

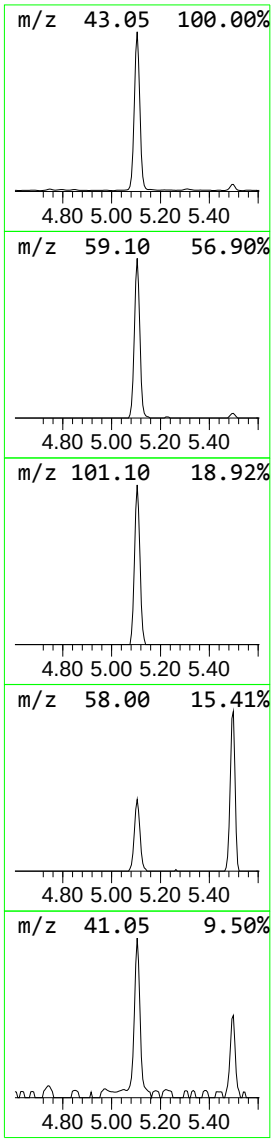
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	4.36 ng	165098	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

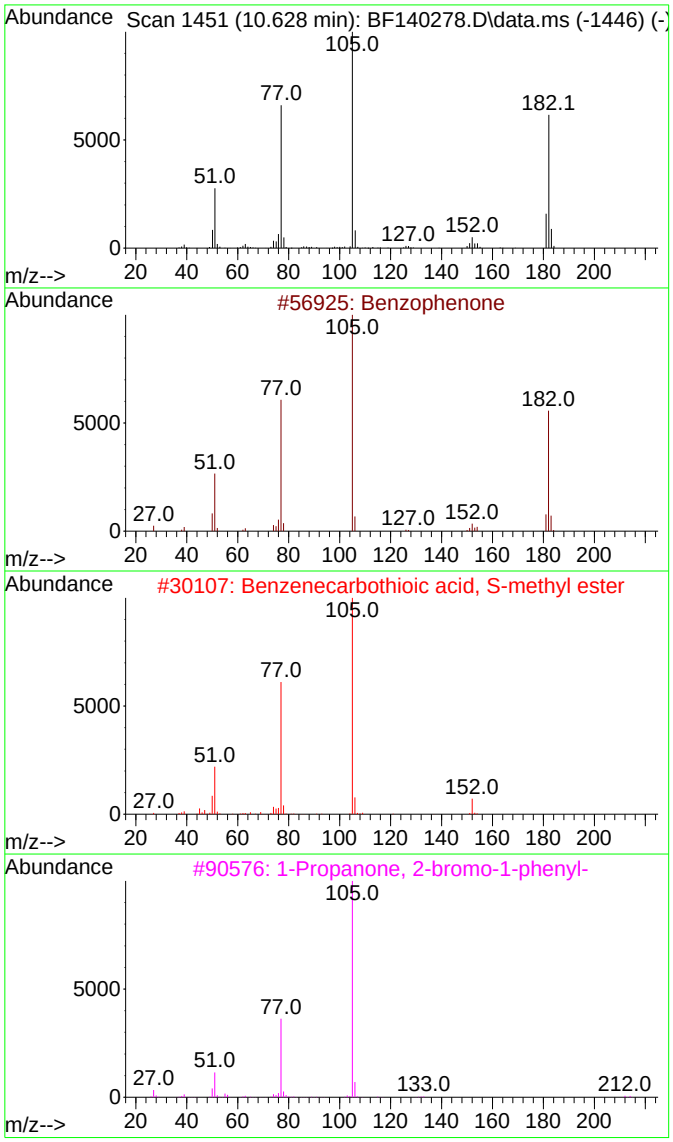
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

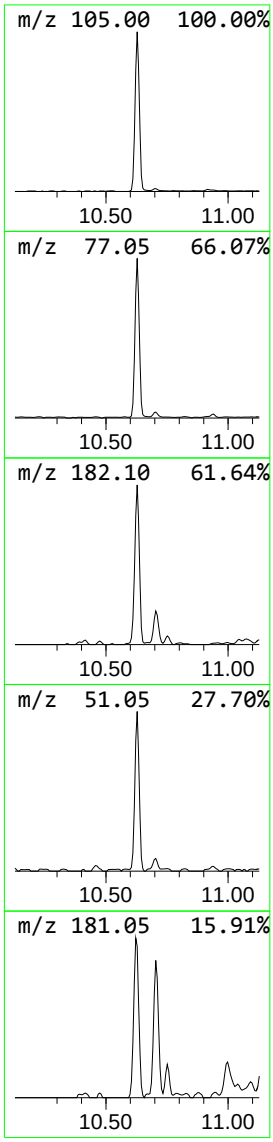
****

Peak Number 4 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.628	5.13 ng	268577	Acenaphthene-d10	9.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	.beta.-Benzilmonoxime	225	C14H11NO2	014090-77-8	47
5	Methyl benzilate	242	C15H14O3	000076-89-1	47





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ALS Vial : 19 Sample Multiplier: 1

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

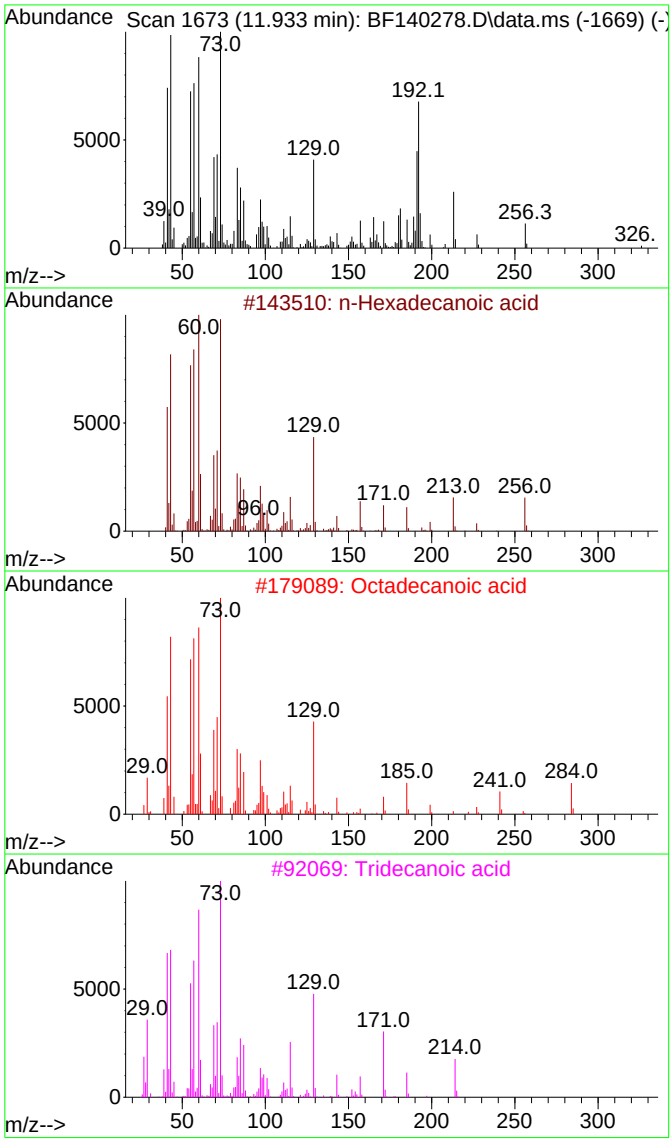
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

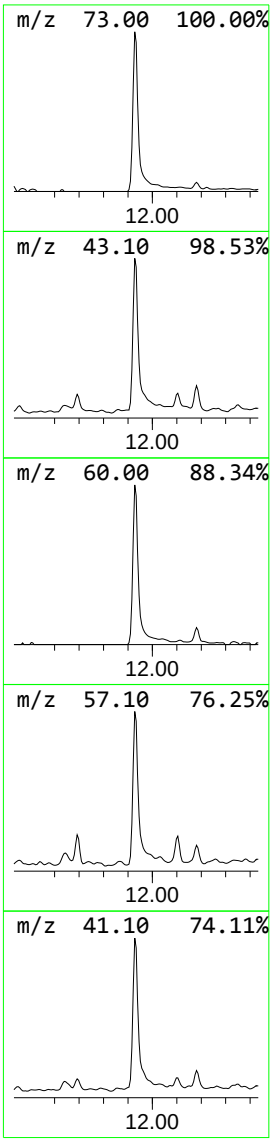
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	7.98 ng	381076	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	92
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	70





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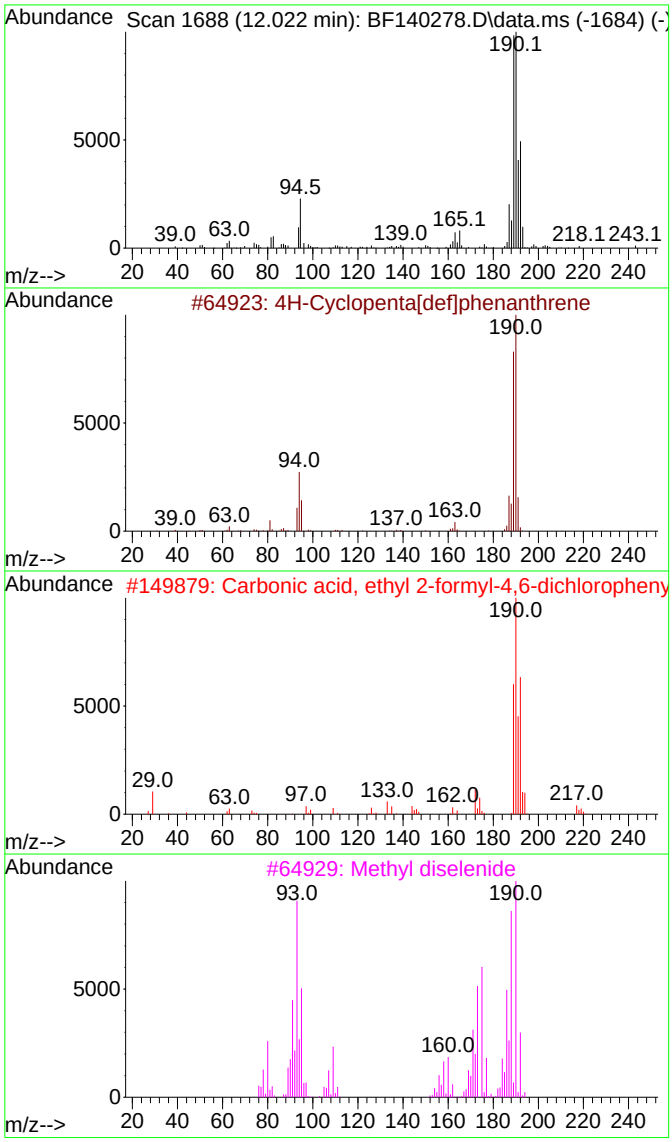
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

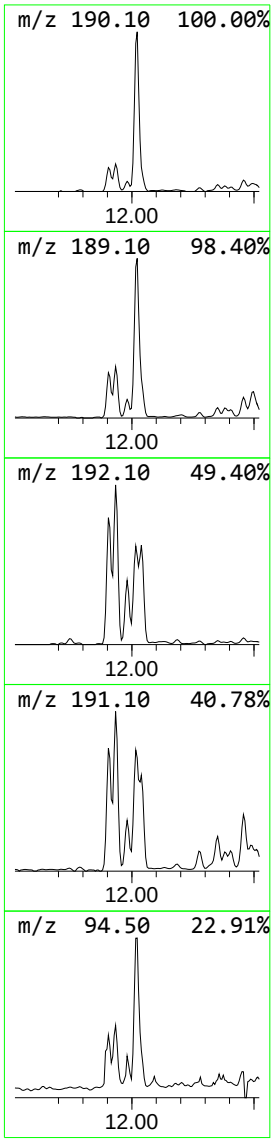
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.022	6.44 ng	307494	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	92
2	Carbonic acid, ethyl 2-formyl-4,...	262	C10H8Cl2O4	1000331-34-4	50
3	Methyl diselenide	190	C2H6Se2	007101-31-7	43
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	40
5	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	40





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Data File : BF140278.D
Acq On : 07 Nov 2024 16:39
Operator : RC/JU
Sample : P4694-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Z-04

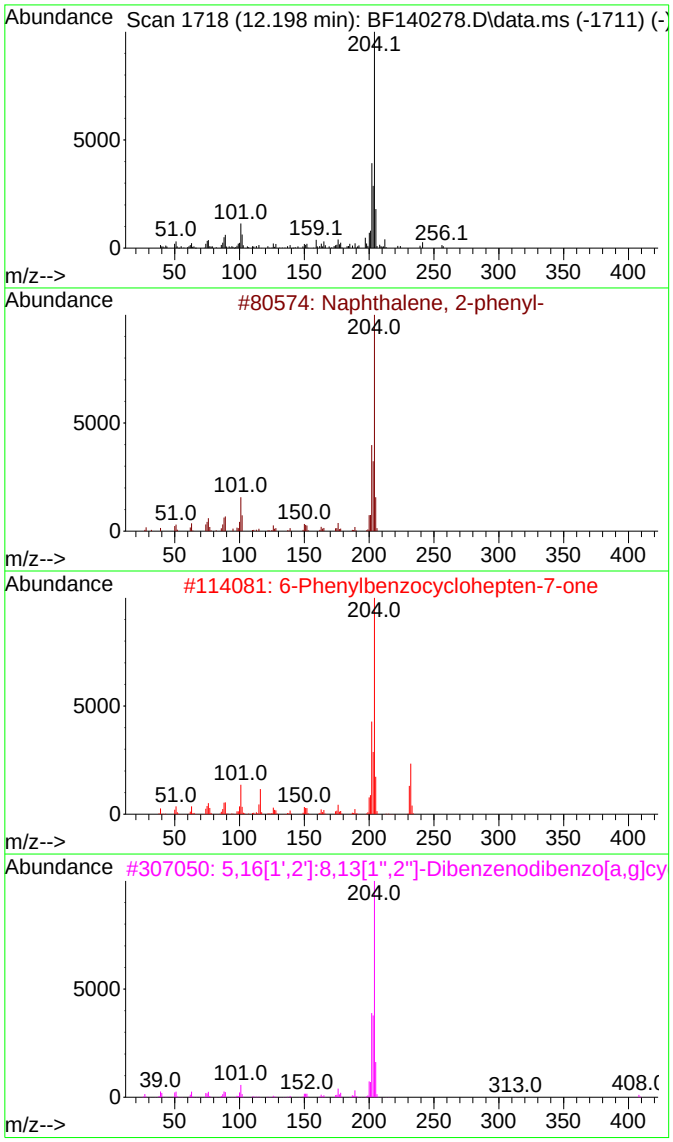
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

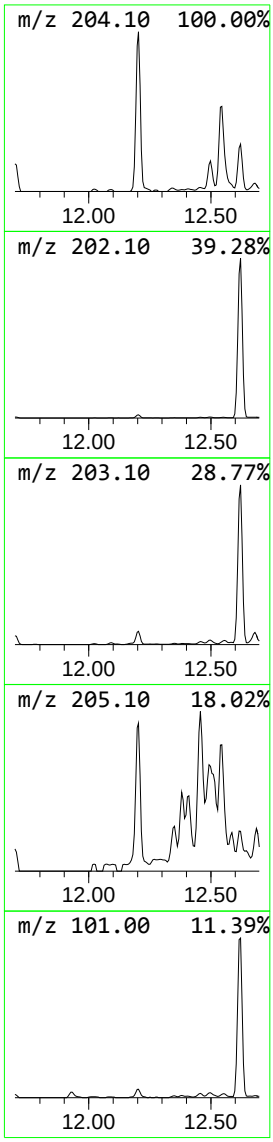
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 2-phenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.198	2.77 ng	132479	Phenanthrene-d10	11.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	93
2	6-Phenylbenzocyclohepten-7-one	232	C17H12O	093327-56-1	90
3	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	86
4	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	70
5	9,10-Bis(bromomethyl)anthracene	362	C16H12Br2	034373-96-1	64





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Acq On : 07 Nov 2024 16:39
Operator : RC/JU
Sample : P4694-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Z-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.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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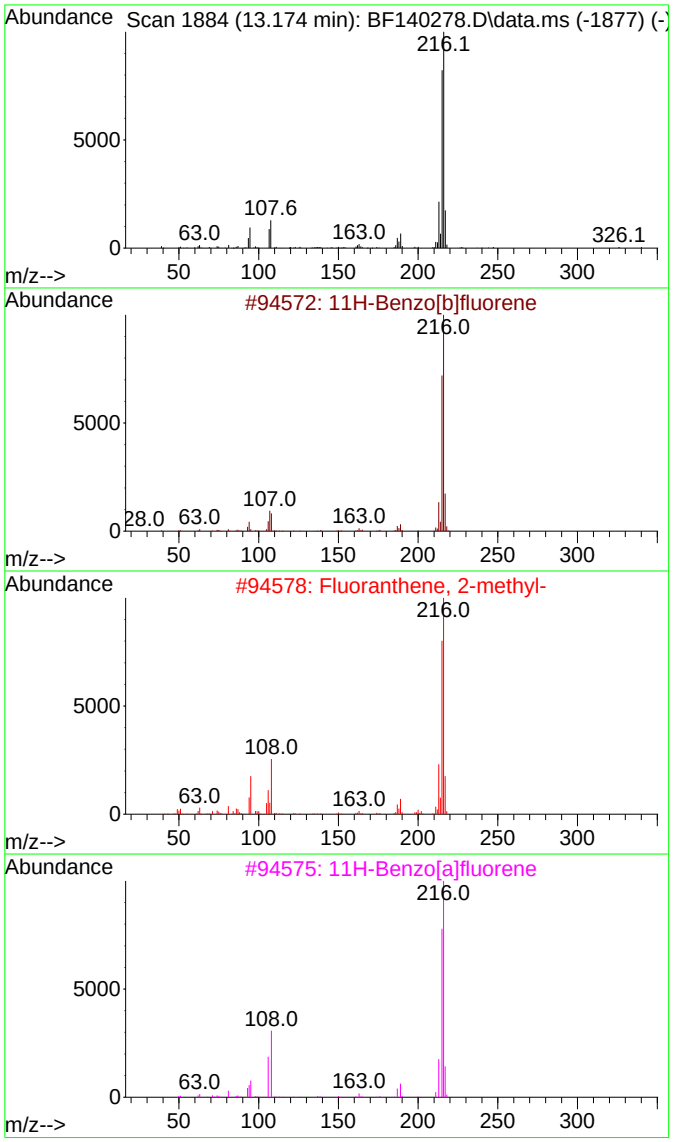
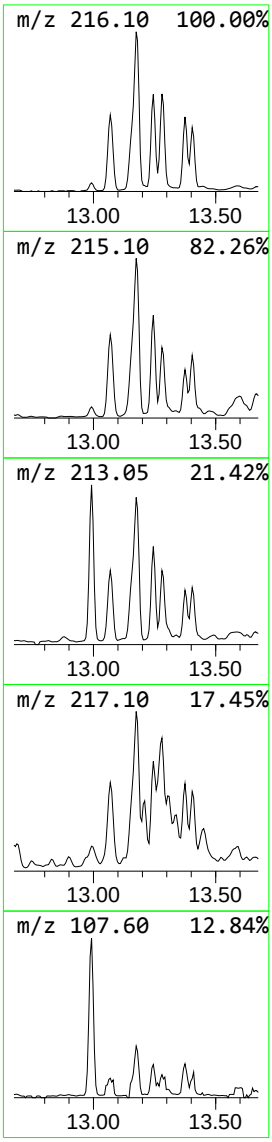
Peak Number 8 11H-Benzo[b]fluorene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.174	2.75 ng	229750	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	95
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	95
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	91
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	87





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Operator : RC/JU
Sample : P4694-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Z-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.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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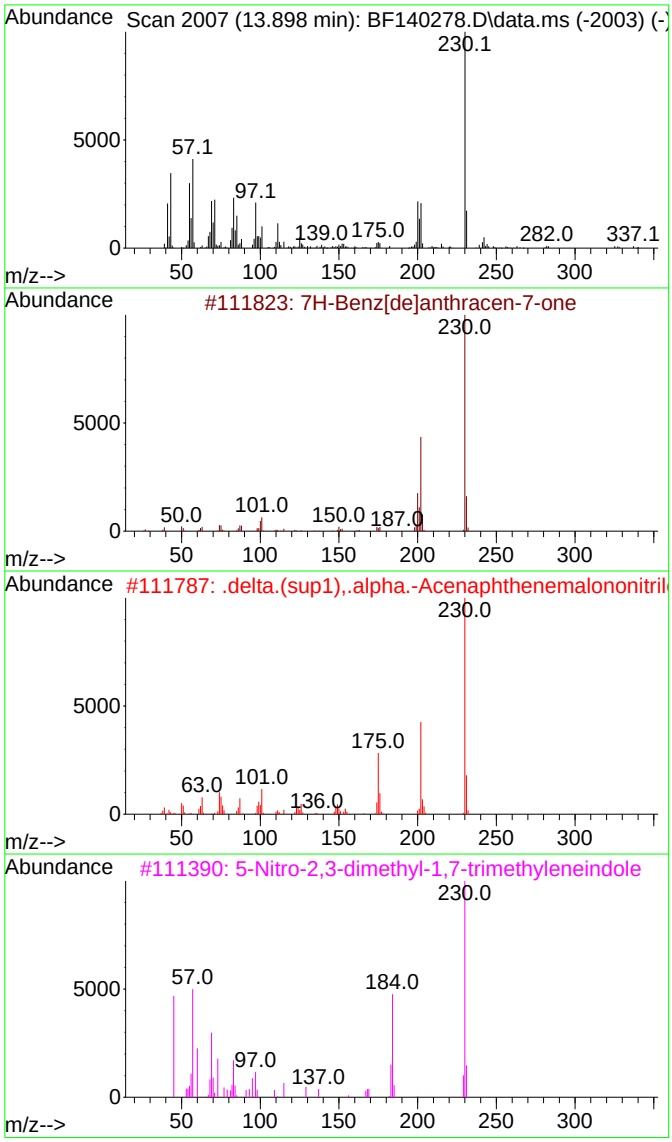
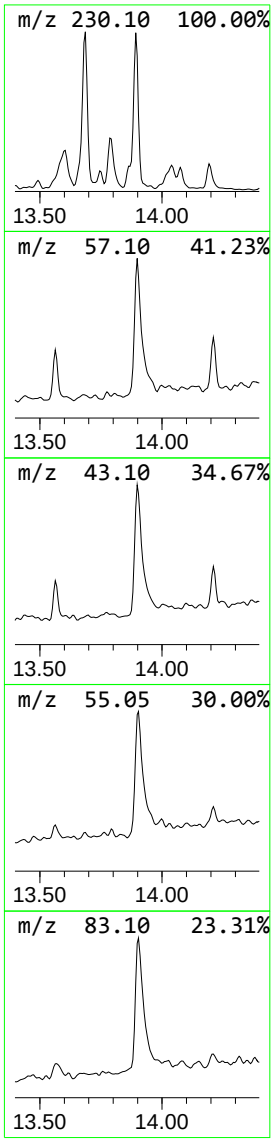
Peak Number 9 7H-Benz[de]anthracen-7-one Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	2.61 ng	217765	Chrysene-d12	14.051

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	90
2	.delta.(sup1),.alpha.-Acenaphthe...	230	C15H6N2O	014619-86-4	43
3	5-Nitro-2,3-dimethyl-1,7-trimeth...	230	C13H14N2O2	003480-19-1	43
4	1-Pyrenecarboxaldehyde	230	C17H10O	003029-19-4	40
5	o-Terphenyl	230	C18H14	000084-15-1	38





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Operator : RC/JU
Sample : P4694-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.M
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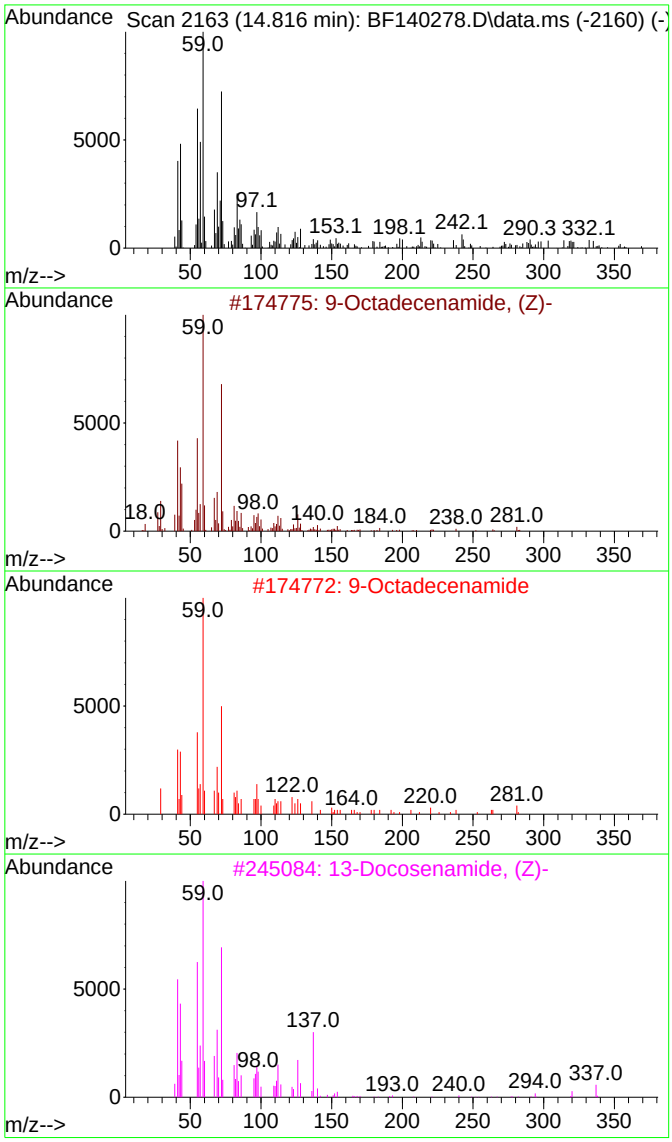
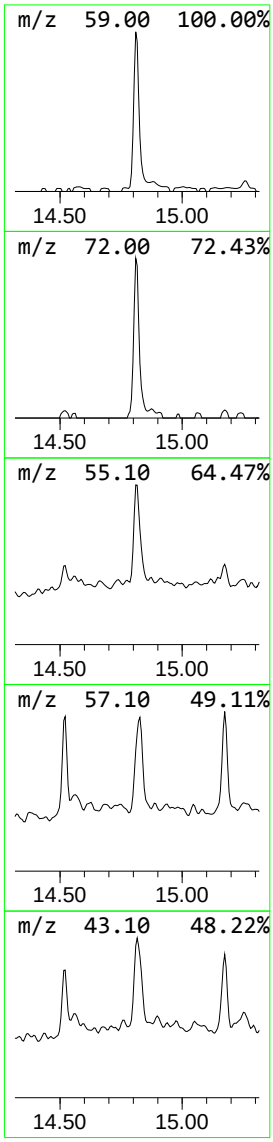
Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	2.71 ng	97680	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2	9-Octadecenamide	281	C18H35NO	003322-62-1	64
3	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	43
4	7-Nonenamide	155	C9H17NO	090949-53-4	22
5	3-((2-Ethoxycarbonyl)-3-methyl-1...	335	C18H25NO5	279231-65-1	14





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Sample : P4694-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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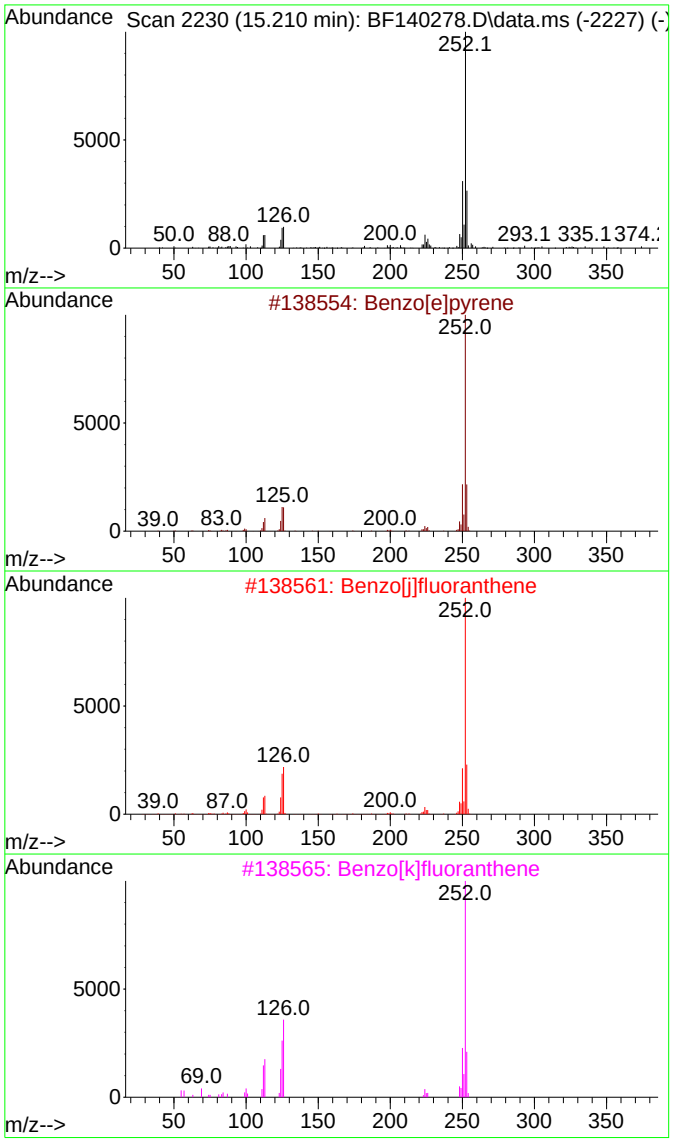
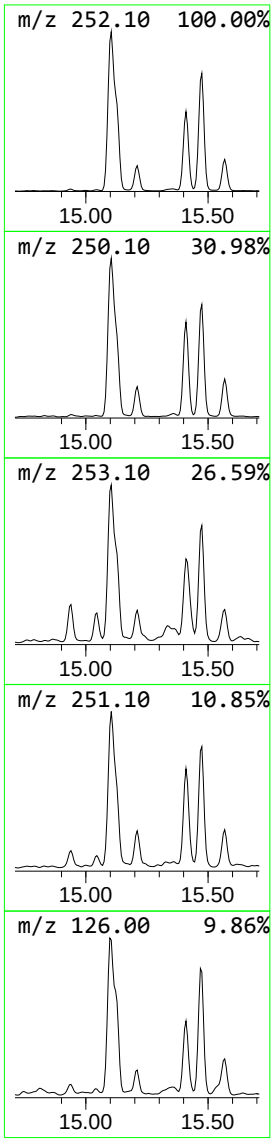
Peak Number 11 Benzo[e]pyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.210	2.01 ng	72342	Perylene-d12	15.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	91
2	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	87
4	Benzo[a]pyrene	252	C20H12	000050-32-8	81
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	81





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Acq On : 07 Nov 2024 16:39
Operator : RC/JU
Sample : P4694-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
Z-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF110524.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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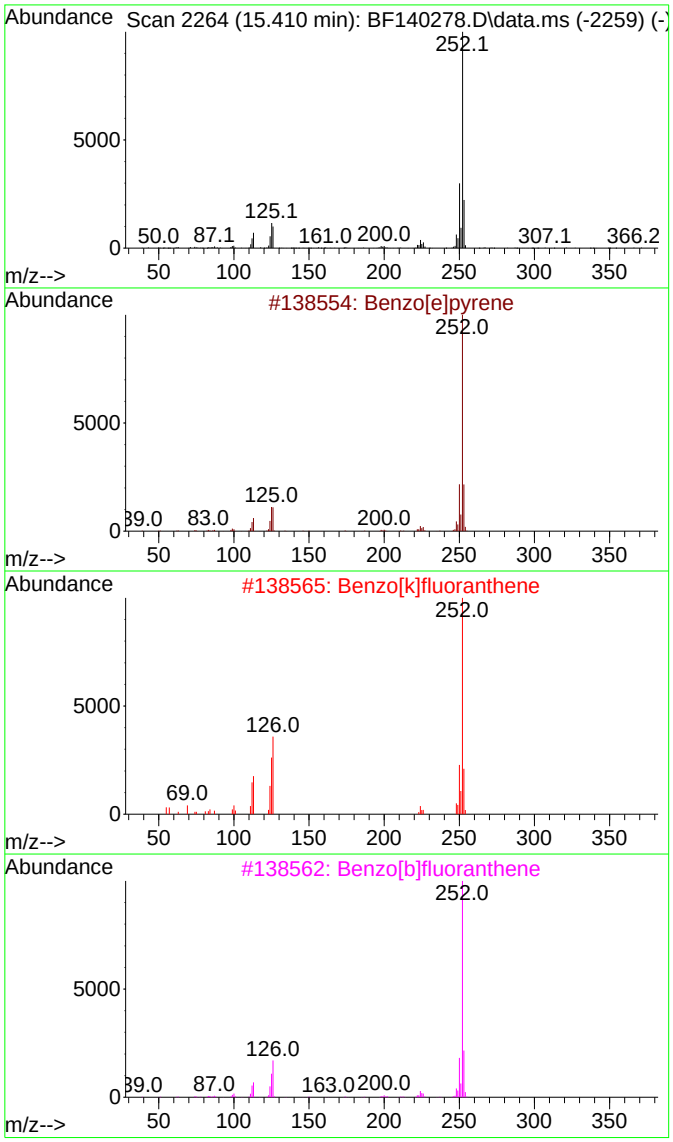
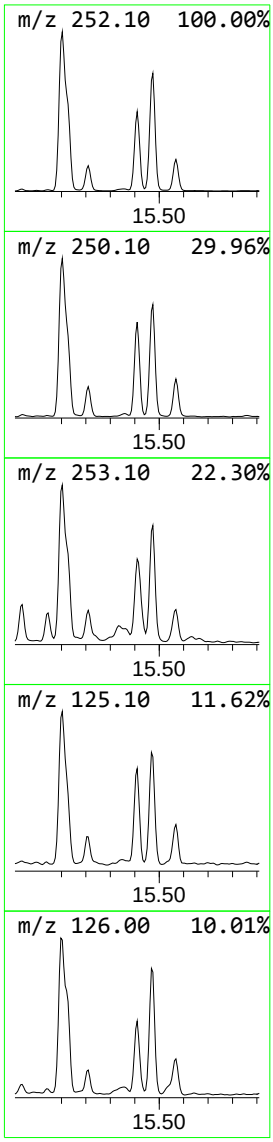
Peak Number 12 Benzo[j]fluoranthene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	8.94 ng	321816	Perylene-d12	15.539

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





Tentatively Identified Compound (LSC) summary

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Operator : RC/JU
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Misc :
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Instrument :
BNA_F
ClientSampleId :
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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...	2.175	48.6	ng	1838450	1	6.875	757171	20.0
Propane, 1,1-di...	2.287	2.0	ng	75760	1	6.875	757171	20.0
2-Pentanone, 4-...	5.104	4.4	ng	165098	1	6.875	757171	20.0
Benzophenone	10.628	5.1	ng	268577	3	9.916	1047390	20.0
n-Hexadecanoic ...	11.933	8.0	ng	381076	4	11.404	955301	20.0
4H-Cyclopenta[d...	12.022	6.4	ng	307494	4	11.404	955301	20.0
Naphthalene, 2-...	12.198	2.8	ng	132479	4	11.404	955301	20.0
11H-Benzo[b]flu...	13.174	2.8	ng	229750	5	14.051	1668260	20.0
7H-Benz[de]anth...	13.898	2.6	ng	217765	5	14.051	1668260	20.0
9-Octadecenamid...	14.816	2.7	ng	97680	6	15.539	720307	20.0
Benzo[e]pyrene	15.210	2.0	ng	72342	6	15.539	720307	20.0
Benzo[j]fluoran...	15.410	8.9	ng	321816	6	15.539	720307	20.0