LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008267.D
Acq On : 08 Dec 2021 00:36
Operator : CG/JU
Sample : M4947-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
355-994

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_P\Methods\8270E-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008267.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.375	400	406	421	rBV	1060831	1554374	47.83%	7.305%
2	6.969	669	677	694	rBV	910820	1564034	48.12%	7.351%
3	7.781	807	815	824	rBV	226450	350954	10.80%	1.649%
4	8.152	870	878	887	rVB	21591	35564	1.09%	0.167%
5	8.946	1005	1013	1023	rBV	557078	979305	30.13%	4.603%
6	10.387	1251	1258	1266	rBV	15219	36654	1.13%	0.172%
7	10.581	1284	1291	1296	rBV	254071	447334	13.76%	2.102%
8	10.628	1296	1299	1308	rVB	31270	51192	1.58%	0.241%
9	12.246	1566	1574	1582	rBV	50664	86448	2.66%	0.406%
10	12.469	1607	1612	1618	rVB	28102	47370	1.46%	0.223%
11	13.051	1703	1711	1722	rBV	1318541	2012794	61.93%	9.460%
12	13.263	1741	1747	1753	rBV3	28934	49613	1.53%	0.233%
13	13.751	1825	1830	1835	rBV3	19138	37452	1.15%	0.176%
14	14.093	1883	1888	1894	rBV4	19203	37204	1.14%	0.175%
15	14.434	1938	1946	1952	rVV	367897	580578	17.86%	2.729%
16	14.493	1952	1956	1965	rVB	95947	151691	4.67%	0.713%
17	14.834	2008	2014	2022	rBV	77267	116975	3.60%	0.550%
18	15.240	2078	2083	2089	rBV2	16065	33756	1.04%	0.159%
19	15.487	2120	2125	2136	rVB	91570	141306	4.35%	0.664%
20	15.787	2171	2176	2183	rBV2	21765	38479	1.18%	0.181%
21	15.934	2194	2201	2208	rBV	1090317	1634885	50.30%	7.684%
22	16.163	2235	2240	2248	rVB6	21996	48364	1.49%	0.227%
23	17.010	2380	2384	2391	rVB2	28077	45705	1.41%	0.215%
24	17.122	2398	2403	2408	rBV2	35979	47017	1.45%	0.221%
25	17.192	2409	2415	2419	rVV	491353	715042	22.00%	3.361%
26	17.234	2419	2422	2429	rVV	214866	317930	9.78%	1.494%
27	17.328	2433	2438	2445	rVB	107429	163611	5.03%	0.769%
28	17.392	2445	2449	2454	rBV	37913	65322	2.01%	0.307%
29	17.610	2482	2486	2493	rVB	30971	47380	1.46%	0.223%
30	17.710	2499	2503	2510	rBV5	14350	33096	1.02%	0.156%
31	18.069	2559	2564	2566	rBV3	20749	34451	1.06%	0.162%
32	18.098	2566	2569	2571	rBV	41979	54887	1.69%	0.258%
33	18.257	2591	2596	2601	rBV2	81715	139420	4.29%	0.655%
34	18.557	2643	2647	2651	rBV	27908	34978	1.08%	0.164%
35	19.104	2736	2740	2745	rBV	62305	84996	2.62%	0.399%
36	19.216	2754	2759	2765	rBV	639788	813242	25.02%	3.822%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008267.D
Acq On : 08 Dec 2021 00:36
Operator : CG/JU
Sample : M4947-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
355-994

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_P\Methods\8270E-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.269	2765	2768	2772	rVB2	44101	60205	1.85%	0.283%
38	19.569	2810	2819	2828	rVB	561928	889568	27.37%	4.181%
39	19.769	2847	2853	2858	rBV	2735132	3250080	100.00%	15.275%
40	20.057	2898	2902	2907	rVB2	87761	132266	4.07%	0.622%
41	20.151	2915	2918	2923	rVB	81542	99821	3.07%	0.469%
42	20.975	3054	3058	3062	rBV	110491	204305	6.29%	0.960%
43	21.022	3062	3066	3072	rVV2	313298	603697	18.57%	2.837%
44	21.080	3072	3076	3083	rVB	688845	821063	25.26%	3.859%
45	21.298	3107	3113	3117	rBV2	819456	1278336	39.33%	6.008%
46	21.339	3117	3120	3129	rVB	189562	280295	8.62%	1.317%
47	23.698	3515	3521	3527	rVB2	515752	1024510	31.52%	4.815%

Sum of corrected areas: 21277549

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Instrument :
BNA_P
ClientSampleId :
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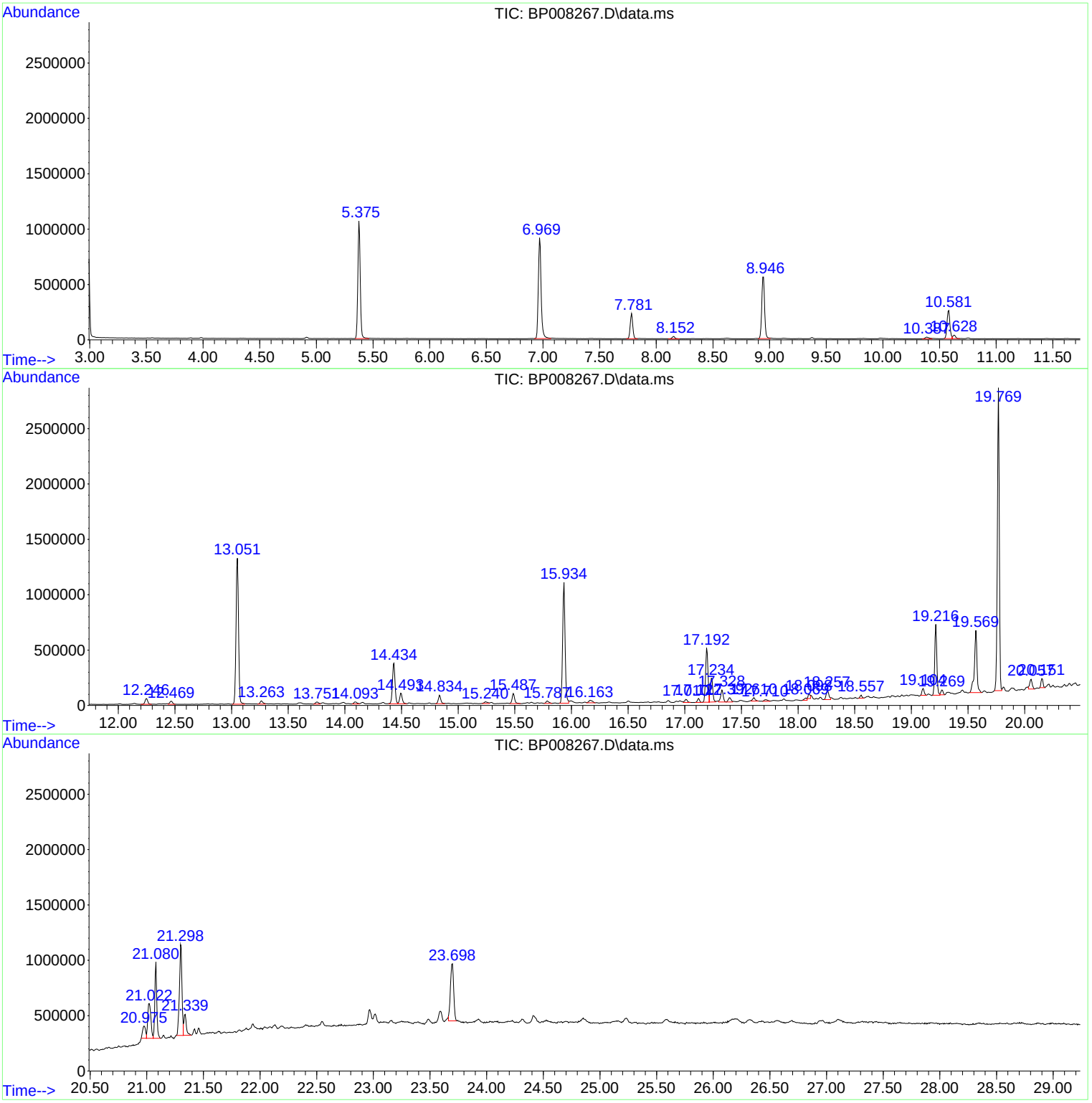
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008267.D
Acq On : 08 Dec 2021 00:36
Operator : CG/JU
Sample : M4947-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

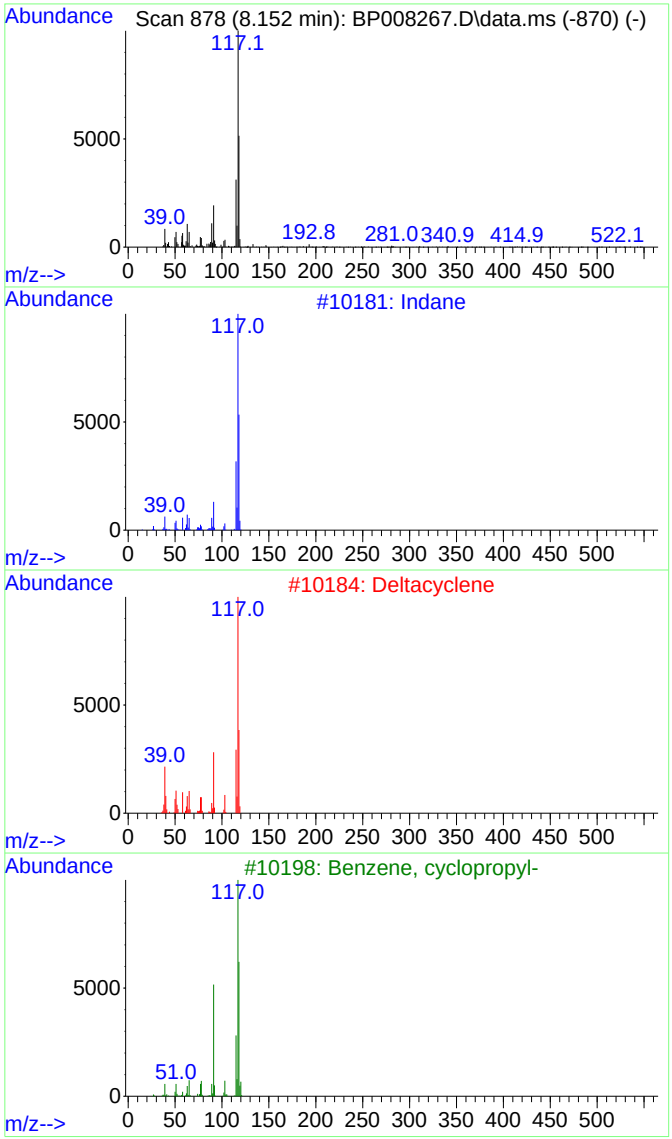
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

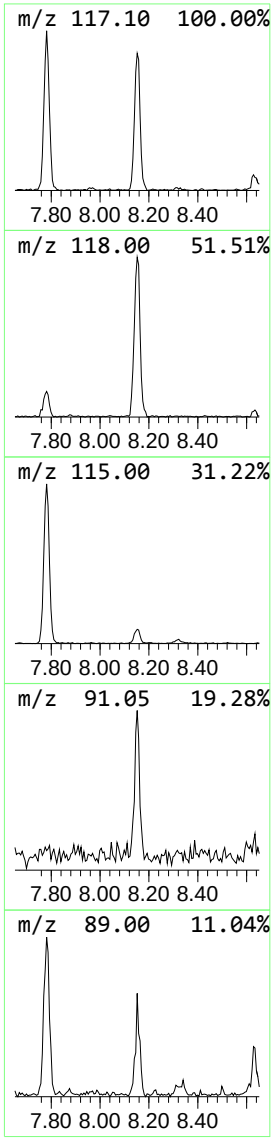
****

Peak Number 1 Indane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.152	2.03 ng	35564	1,4-Dichlorobenzene-d4	7.781

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	94
2	Deltacyclene	118	C9H10	007785-10-6	76
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
5	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	62





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Data File : BP008267.D
Acq On : 08 Dec 2021 00:36
Operator : CG/JU
Sample : M4947-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
355-994

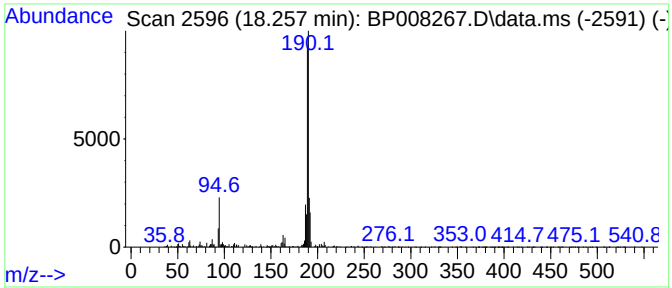
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

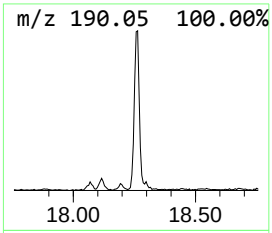
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

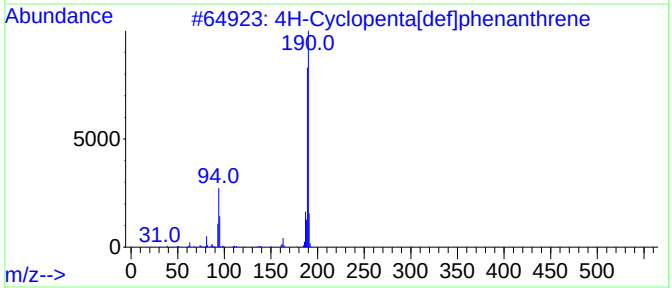
****
Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

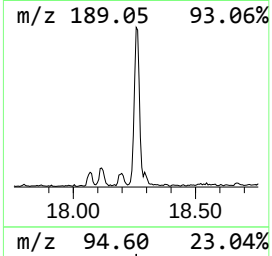
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.257	3.90 ng	139420	Phenanthrene-d10	17.192

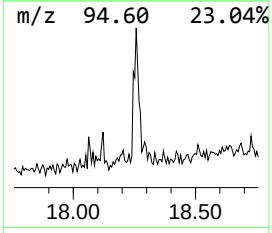
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
3	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	17
4	Methyl diselenide	190	C2H6Se2	007101-31-7	16
5	2-Naphthaldehyde, 1,2,3,4-tetrah...	190	C12H14O2	002472-02-8	14

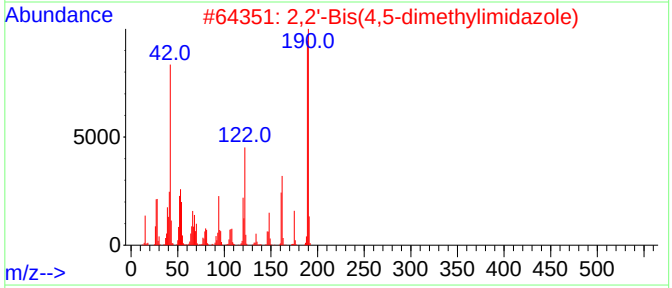


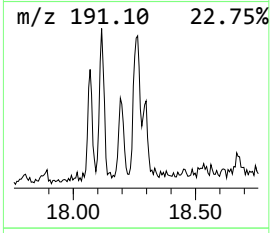


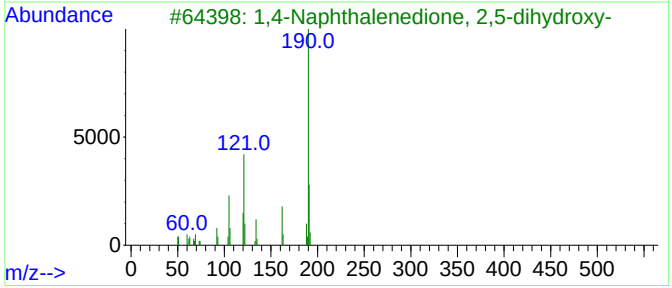


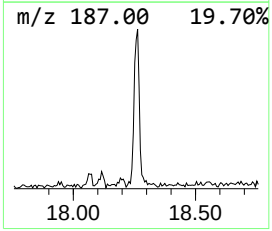












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008267.D
Acq On : 08 Dec 2021 00:36
Operator : CG/JU
Sample : M4947-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
355-994

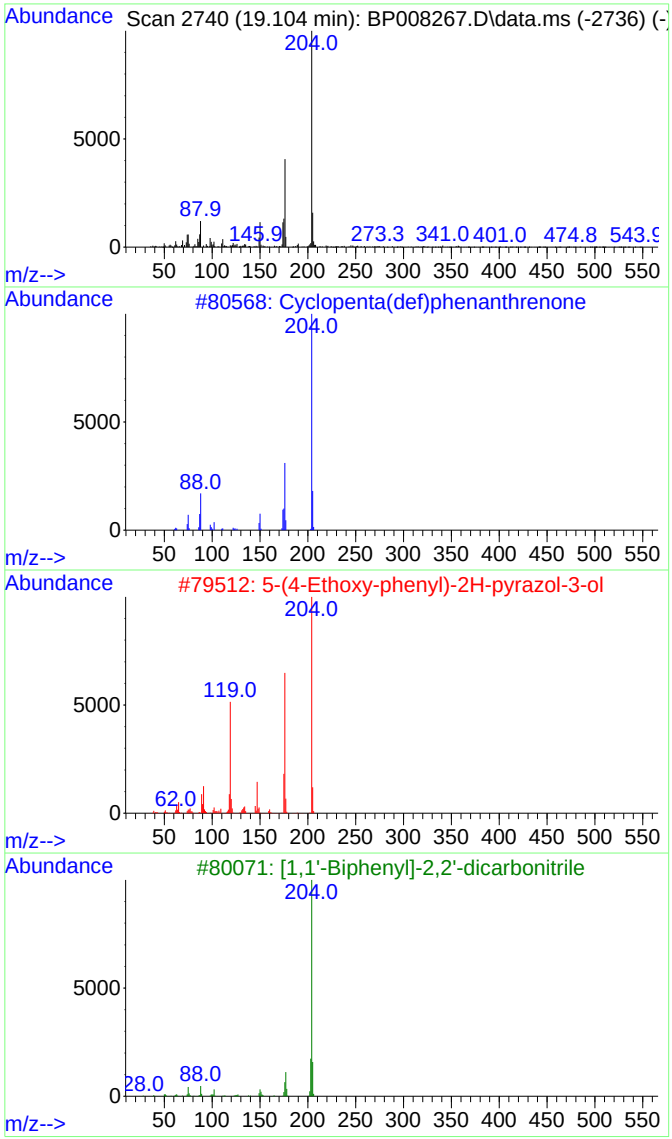
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

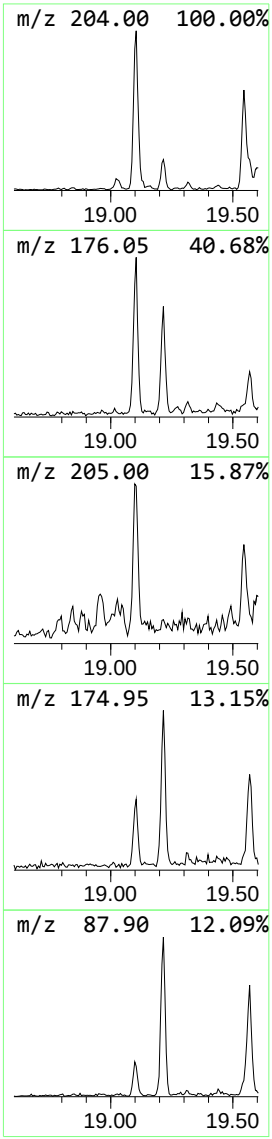
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopenta(def)phenanthrenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.104	2.38 ng	84996	Phenanthrene-d10	17.192

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	94
2	5-(4-Ethoxy-phenyl)-2H-pyrazol-3-ol	204	C11H12N2O2	1000278-26-8	50
3	[1,1'-Biphenyl]-2,2'-dicarbonitrile	204	C14H8N2	004341-02-0	50
4	Tetracyano-p-quinodimethane	204	C12H4N4	001518-16-7	46
5	[1,2,4]Triazolo[5,1-b]quinazolin...	204	C10H12N4O	1000337-56-5	45





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Operator : CG/JU
Sample : M4947-01
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
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TIC Library : C:\Database\NIST20.L
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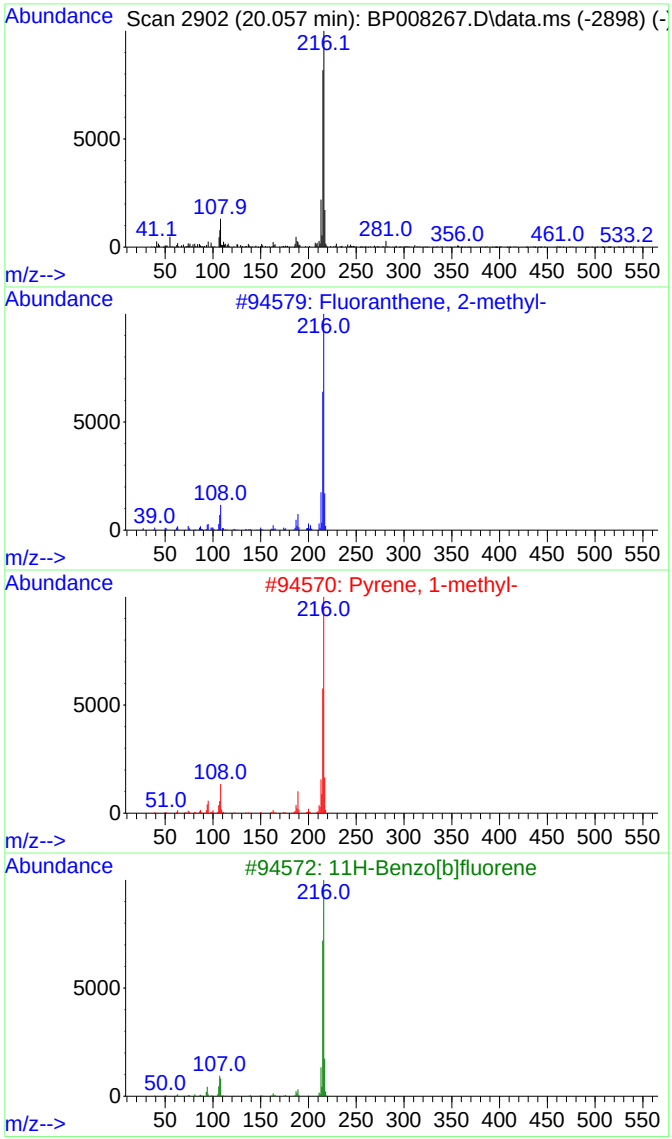
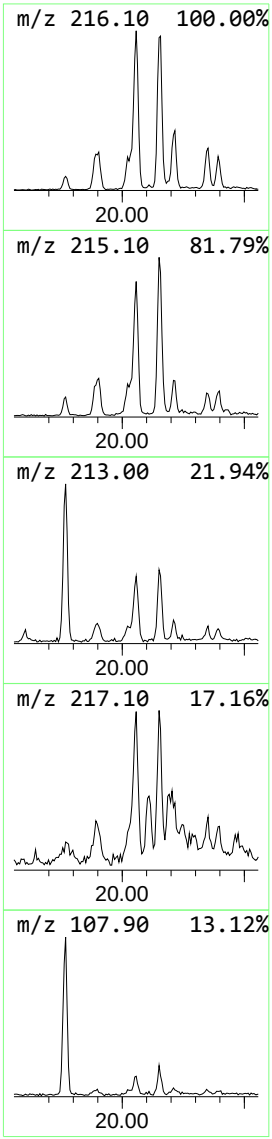
****

Peak Number 5 Fluoranthene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.057	2.07 ng	132266	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
4	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
5	Pyrene, 2-methyl-	216	C17H12	003442-78-2	70





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

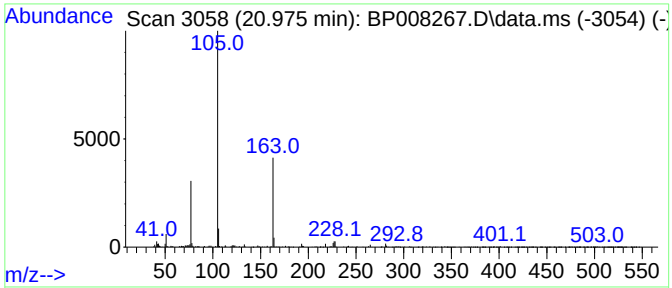
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

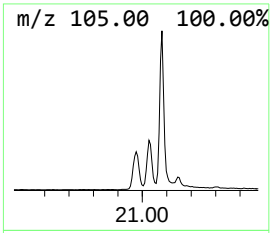
****

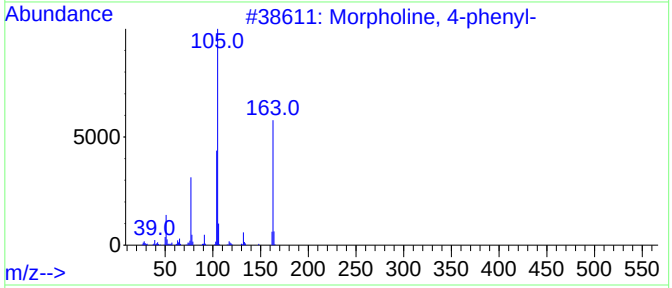
Peak Number 6 Morpholine, 4-phenyl- Concentration Rank 4

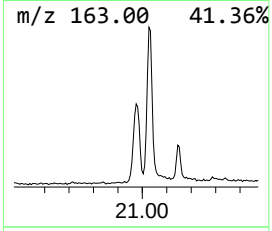
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.974	3.20 ng	204305	Chrysene-d12	21.304

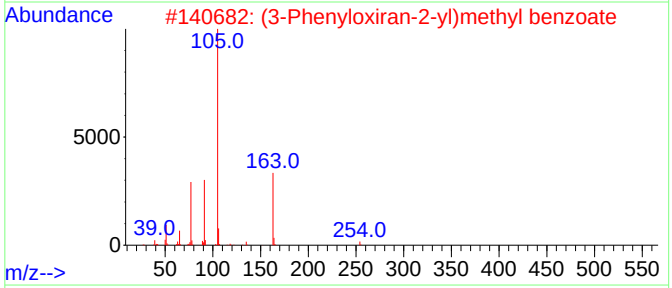
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	56
2	(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	56
3	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	40
4	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	40
5	3-Benzoylaminochromone	265	C16H11NO3	1000243-49-5	35

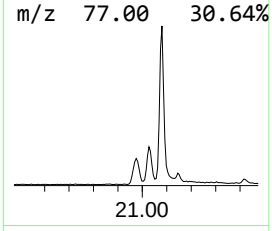


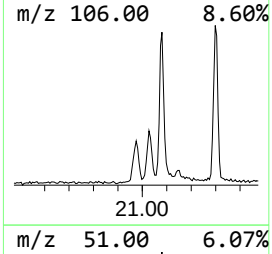


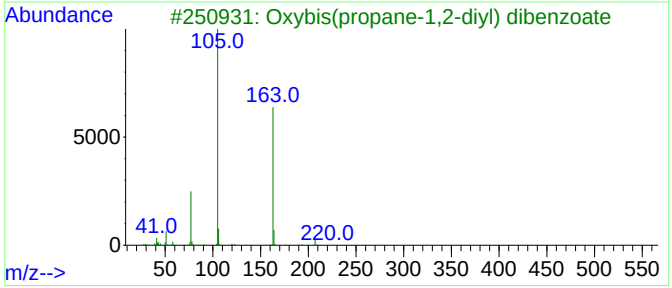


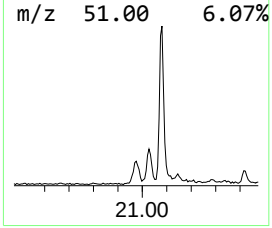












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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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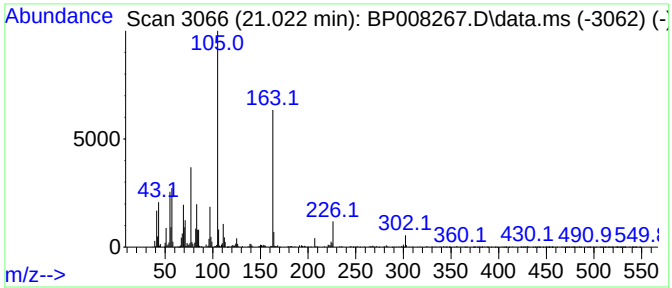
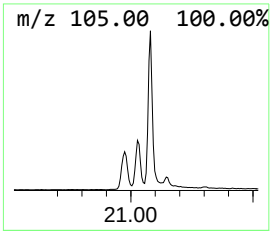
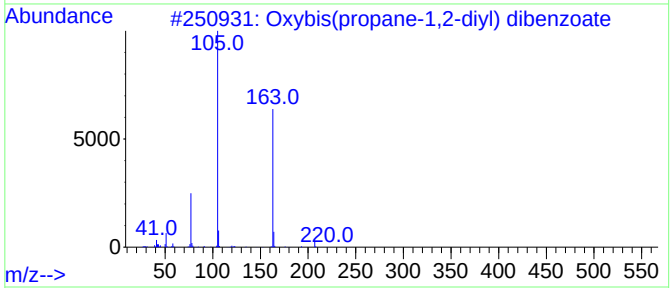
Peak Number 7 unknown21.022 Concentration Rank 2

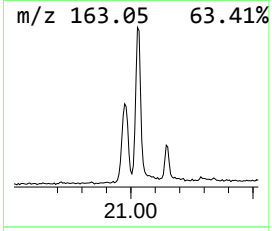
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.022	9.45 ng	603697	Chrysene-d12	21.304

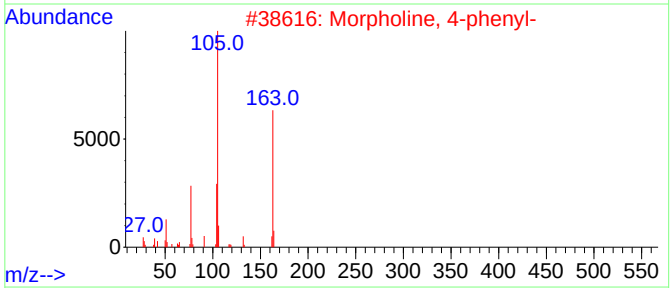
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	46
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	43
3	Benzamide, N-propyl-	163	C10H13NO	010546-70-0	43
4	Benzoic acid, anhydride	226	C14H10O3	000093-97-0	22
5	N-(4-Methoxy-2-nitrophenyl)benza...	272	C14H12N2O4	038259-63-1	22

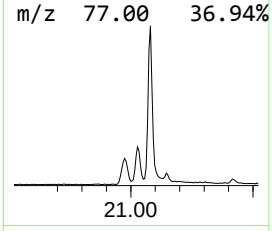


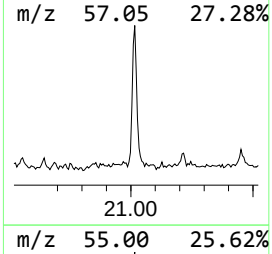


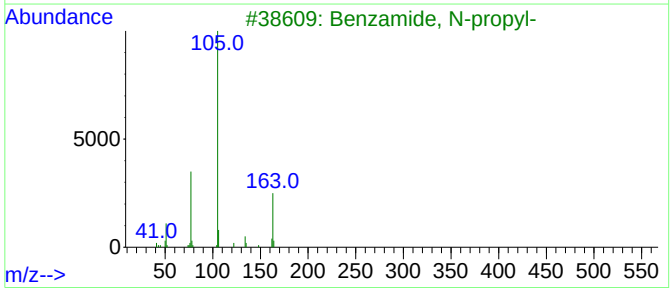


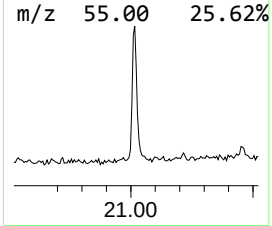












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008267.D
Acq On : 08 Dec 2021 00:36
Operator : CG/JU
Sample : M4947-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
355-994

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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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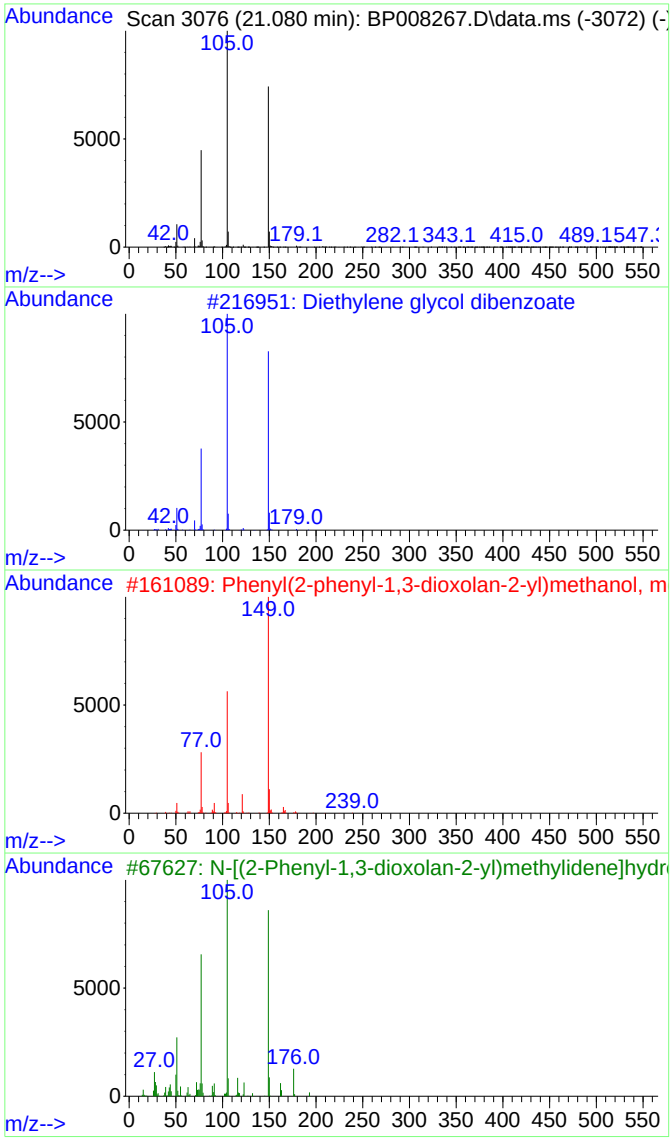
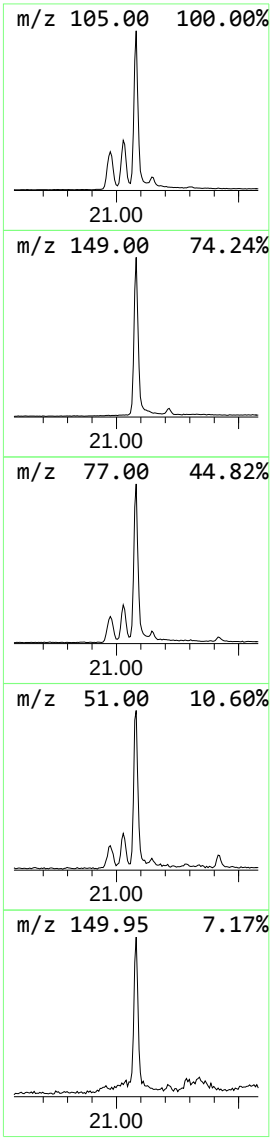
Peak Number 8 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.080	12.85 ng	821063	Chrysene-d12	21.304

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2	Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	78
3	N-[(2-Phenyl-1,3-dioxolan-2-yl)m...	193	C10H11NO3	1000411-48-9	78
4	Phenyl(2-phenyl-1,3-dioxolan-2-y...	298	C18H18O4	006963-16-2	78
5	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120721\
Data File : BP008267.D
Acq On : 08 Dec 2021 00:36
Operator : CG/JU
Sample : M4947-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
355-994

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.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
Indane	8.152	2.0	ng	35564	1	7.781	350954	20.0
4H-Cyclopenta[d...	18.257	3.9	ng	139420	4	17.192	715042	20.0
Cyclopenta(def)...	19.104	2.4	ng	84996	4	17.192	715042	20.0
Fluoranthene, 2...	20.057	2.1	ng	132266	5	21.304	1278340	20.0
Morpholine, 4-p...	20.974	3.2	ng	204305	5	21.304	1278340	20.0
unknown21.022	21.022	9.4	ng	603697	5	21.304	1278340	20.0
Diethylene glyc...	21.080	12.9	ng	821063	5	21.304	1278340	20.0