LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056345.D
Acq On : 19 Jan 2023 2:20
Operator : CG/JU
Sample : 01178-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-011723

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_G\Methods\8270-BG122722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056345.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.321	3	5	14	rVB	79375	108619	6.90%	0.899%
2	5.348	344	350	358	rBV	89020	139316	8.85%	1.153%
3	5.829	425	432	440	rBV	330721	535657	34.03%	4.434%
4	7.445	700	707	716	rBV	336894	595638	37.85%	4.931%
5	8.309	847	854	862	rVB	143661	248439	15.79%	2.057%
6	9.484	1046	1054	1065	rVB	206168	386480	24.56%	3.199%
7	11.076	1318	1325	1328	rBV4	9524	16299	1.04%	0.135%
8	11.141	1329	1336	1343	rVB	188865	339708	21.58%	2.812%
9	12.310	1528	1535	1540	rVB4	10265	16949	1.08%	0.140%
10	12.504	1564	1568	1576	rVB4	12338	19626	1.25%	0.162%
11	13.544	1738	1745	1752	rBV	756380	1175280	74.67%	9.729%
12	13.720	1764	1775	1779	rBV5	15332	27909	1.77%	0.231%
13	14.243	1859	1864	1868	rBV4	12914	23588	1.50%	0.195%
14	14.484	1899	1905	1909	rBV8	12050	21620	1.37%	0.179%
15	14.648	1928	1933	1942	rBV8	7406	18244	1.16%	0.151%
16	14.778	1950	1955	1960	rVB3	12425	18061	1.15%	0.150%
17	14.919	1974	1979	1985	rVB	314544	505484	32.12%	4.185%
18	14.983	1987	1990	1995	rVB2	15179	22264	1.41%	0.184%
19	15.119	2009	2013	2021	rBV4	11366	25217	1.60%	0.209%
20	15.307	2037	2045	2052	rVB5	16755	37081	2.36%	0.307%
21	15.383	2052	2058	2063	rBV2	17487	27059	1.72%	0.224%
22	15.524	2077	2082	2087	rBV6	15184	27840	1.77%	0.230%
23	15.700	2104	2112	2113	rBV6	13663	27201	1.73%	0.225%
24	15.724	2113	2116	2121	rVB4	21478	30230	1.92%	0.250%
25	15.953	2151	2155	2163	rBV7	15520	41754	2.65%	0.346%
26	16.117	2180	2183	2187	rVB6	11509	17216	1.09%	0.143%
27	16.258	2197	2207	2213	rVB	49085	98829	6.28%	0.818%
28	16.399	2226	2231	2238	rVB	450958	705755	44.84%	5.842%
29	16.582	2257	2262	2264	rBV4	17711	27962	1.78%	0.231%
30	16.817	2300	2302	2308	rVB6	14264	22813	1.45%	0.189%
31	17.010	2331	2335	2338	rBV3	13792	20109	1.28%	0.166%
32	17.175	2358	2363	2364	rBV5	9512	17048	1.08%	0.141%
33	17.310	2381	2386	2391	rBV7	17329	36875	2.34%	0.305%
34	17.369	2394	2396	2400	rVV3	11599	16526	1.05%	0.137%
35	17.657	2439	2445	2449	rBV	390930	621288	39.47%	5.143%
36	17.698	2449	2452	2458	rVB	255761	376808	23.94%	3.119%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056345.D
Acq On : 19 Jan 2023 2:20
Operator : CG/JU
Sample : 01178-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-011723

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_G\Methods\8270-BG122722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.792	2464	2468	2472	rVB	61034	81186	5.16%	0.672%
38	18.280	2548	2551	2556	rVB3	18898	22011	1.40%	0.182%
39	18.503	2586	2589	2590	rBV	51710	50975	3.24%	0.422%
40	18.573	2598	2601	2608	rVB	70334	103563	6.58%	0.857%
41	18.726	2620	2627	2630	rBV3	82905	178234	11.32%	1.475%
42	19.008	2672	2675	2680	rBV	51238	76391	4.85%	0.632%
43	19.408	2739	2743	2745	rBV2	98590	130810	8.31%	1.083%
44	19.572	2767	2771	2775	rVB5	30693	54307	3.45%	0.450%
45	19.696	2786	2792	2797	rBV	650295	966459	61.41%	8.001%
46	20.019	2843	2847	2849	rBV2	110877	177026	11.25%	1.465%
47	20.054	2849	2853	2858	rVB	572148	767041	48.74%	6.350%
48	20.230	2878	2883	2889	rBV	1219975	1573883	100.00%	13.029%
49	21.952	3168	3176	3181	rBV2	446366	1191384	75.70%	9.863%
50	22.005	3182	3185	3191	rVB	209455	309766	19.68%	2.564%

Sum of corrected areas: 12079828

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
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Operator : CG/JU
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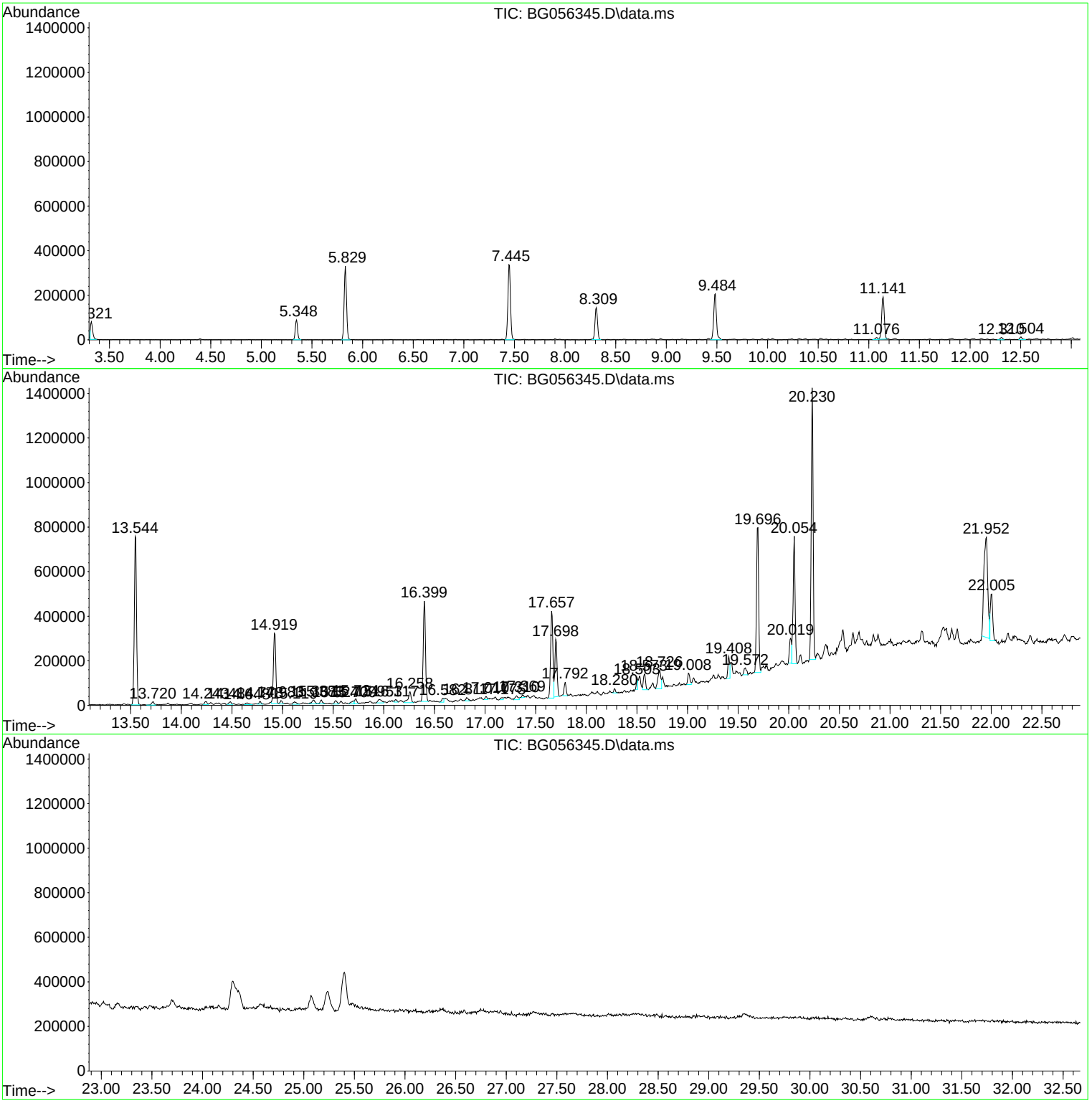
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-011723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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_G\Data\BG011823\
Data File : BG056345.D
Acq On : 19 Jan 2023 2:20
Operator : CG/JU
Sample : 01178-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-011723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

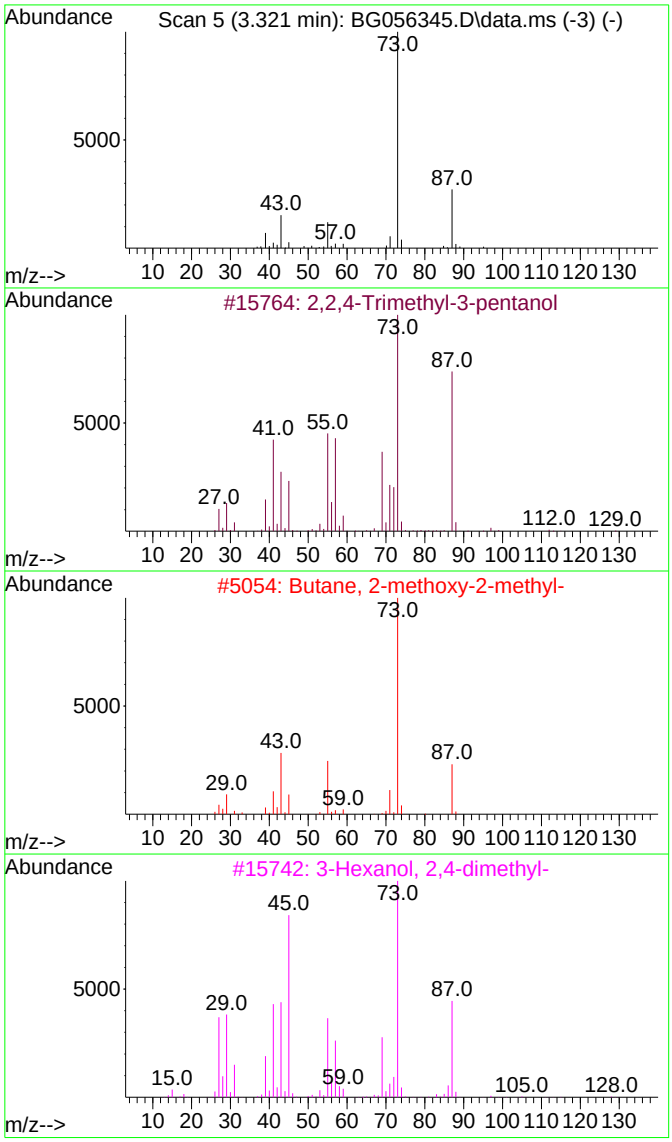
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

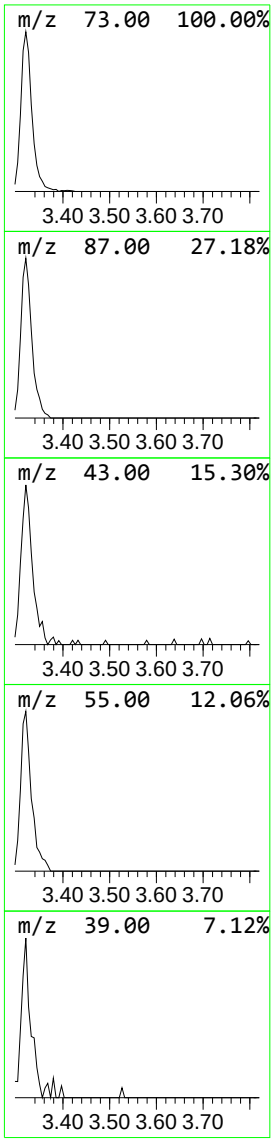
****

Peak Number 1 unknown3.321 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.321	8.74 ng	108619	1,4-Dichlorobenzene-d4	8.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
2	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	38
3	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	36
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056345.D
Acq On : 19 Jan 2023 2:20
Operator : CG/JU
Sample : 01178-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-011723

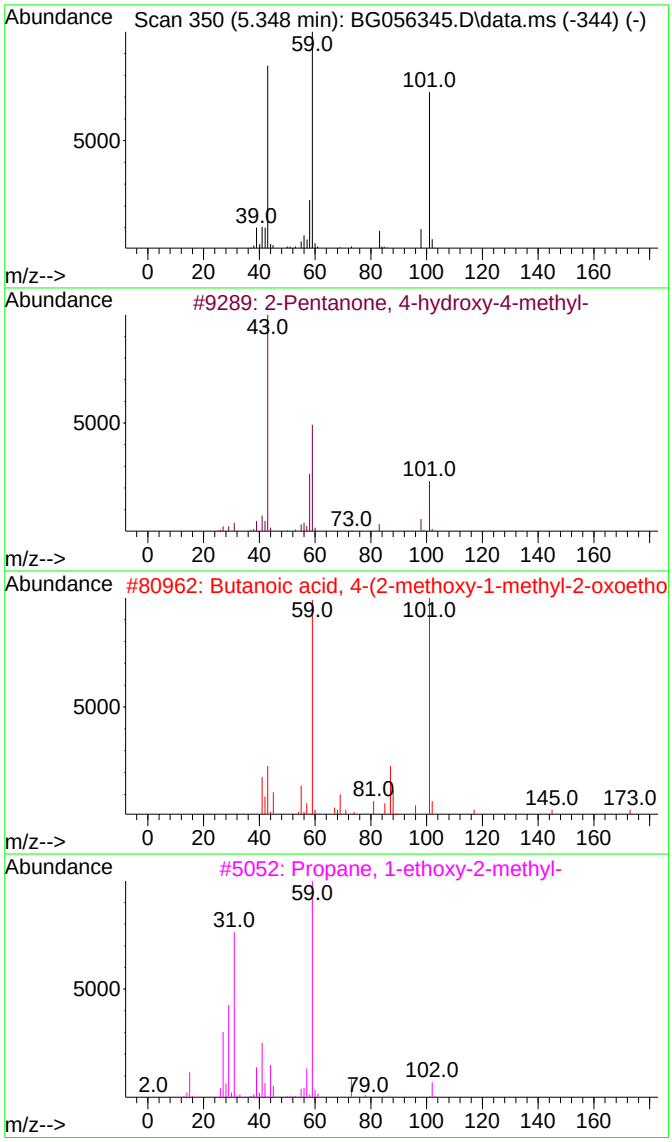
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

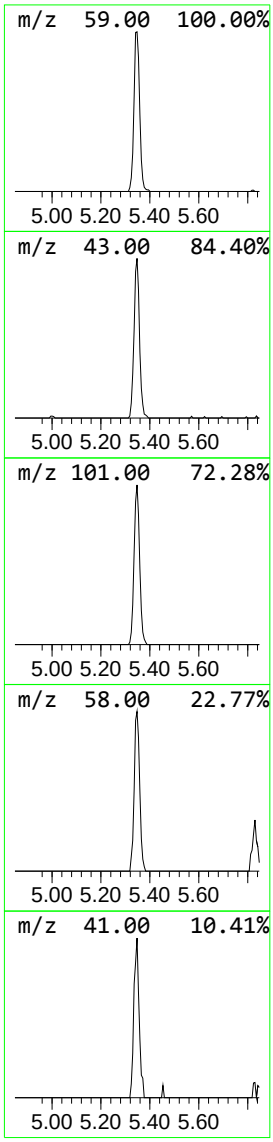
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.348	11.22 ng	139316	1,4-Dichlorobenzene-d4	8.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Butanoic acid, 4-(2-methoxy-1-me...	204	C9H16O5	054966-46-0	36
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056345.D
Acq On : 19 Jan 2023 2:20
Operator : CG/JU
Sample : 01178-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-011723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

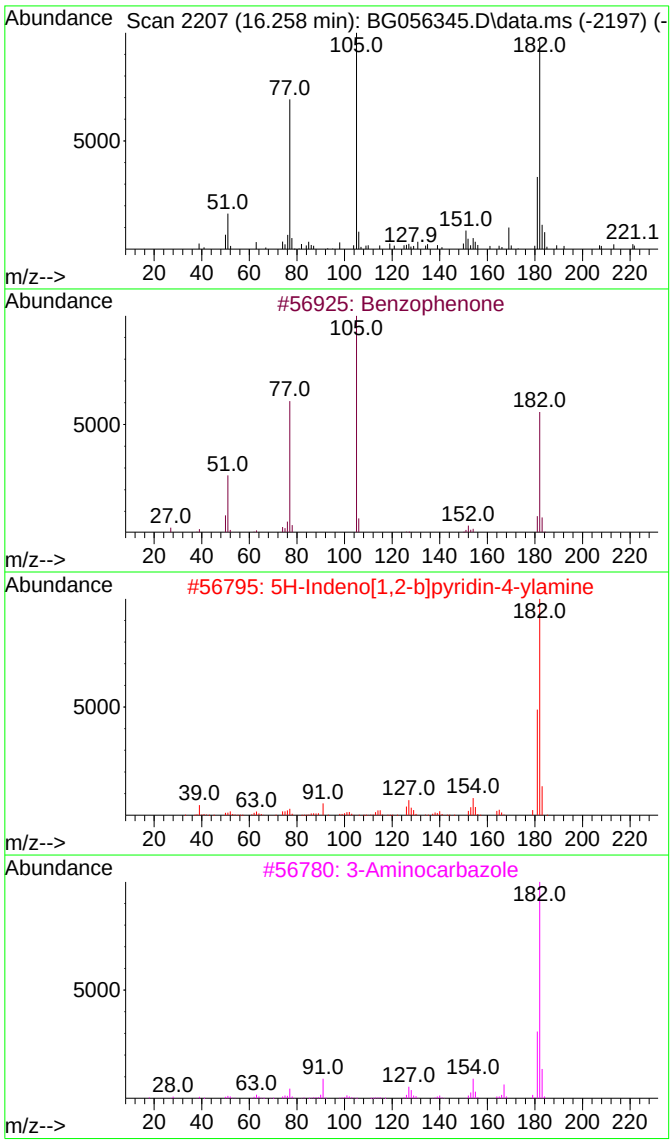
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

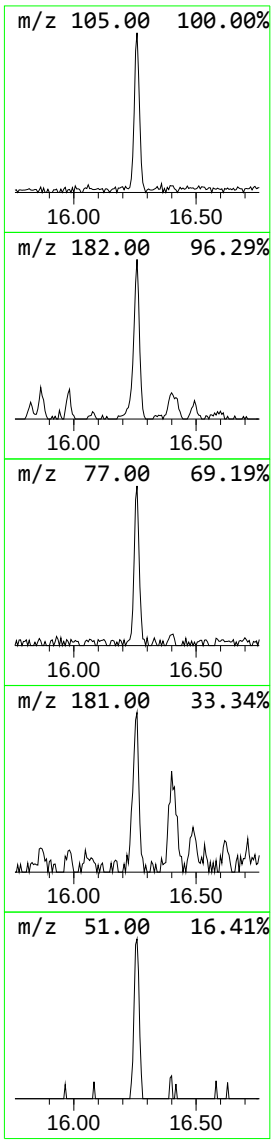
****

Peak Number 3 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.258	3.91 ng	98829	Acenaphthene-d10	14.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	81
2	5H-Indeno[1,2-b]pyridin-4-ylamine	182	C12H10N2	1000303-41-6	46
3	3-Aminocarbazole	182	C12H10N2	006377-12-4	43
4	4,4'-Dimethylbiphenyl	182	C14H14	000613-33-2	43
5	.beta.-Carboline, 2-methyl-	182	C12H10N2	013099-99-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056345.D
Acq On : 19 Jan 2023 2:20
Operator : CG/JU
Sample : 01178-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-011723

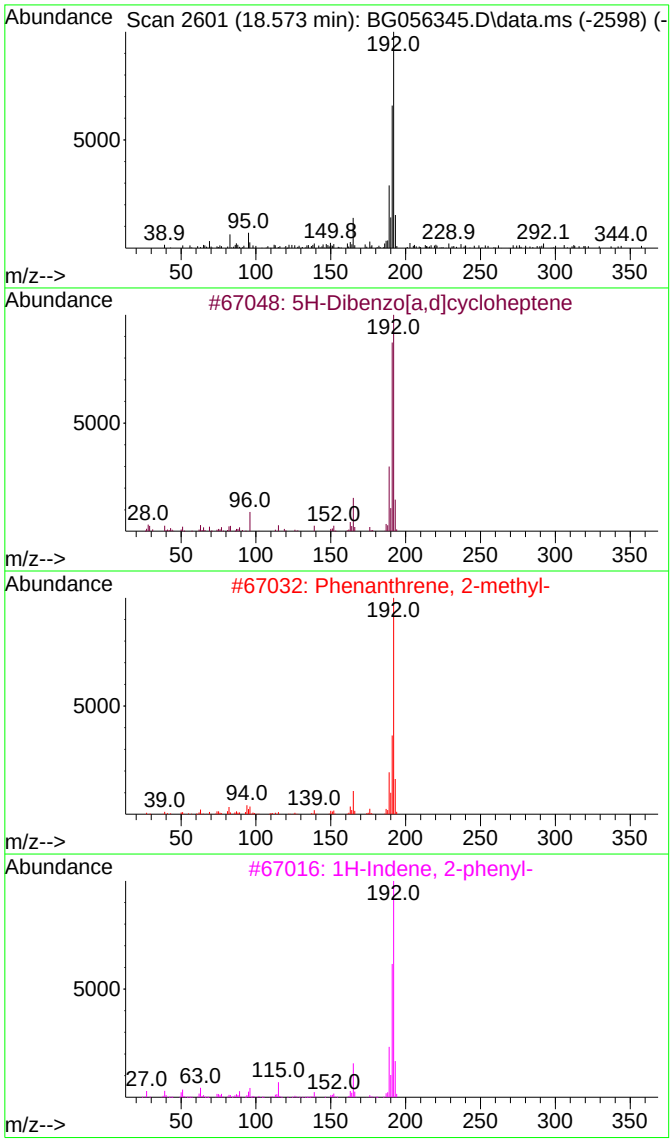
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

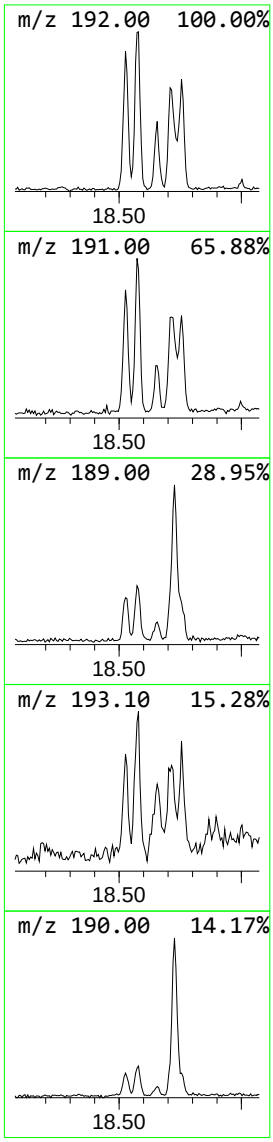
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 5H-Dibenzo[a,d]cycloheptene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.573	3.33 ng	103563	Phenanthrene-d10	17.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	95
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	92
3	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	91
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	90
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056345.D
Acq On : 19 Jan 2023 2:20
Operator : CG/JU
Sample : 01178-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-011723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

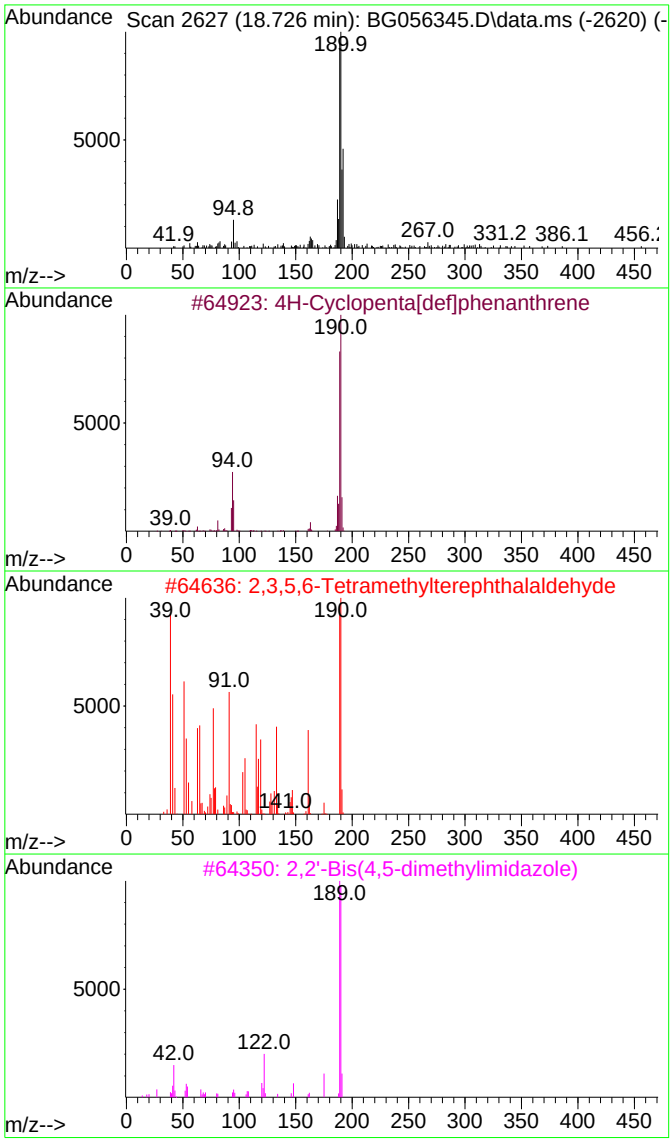
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

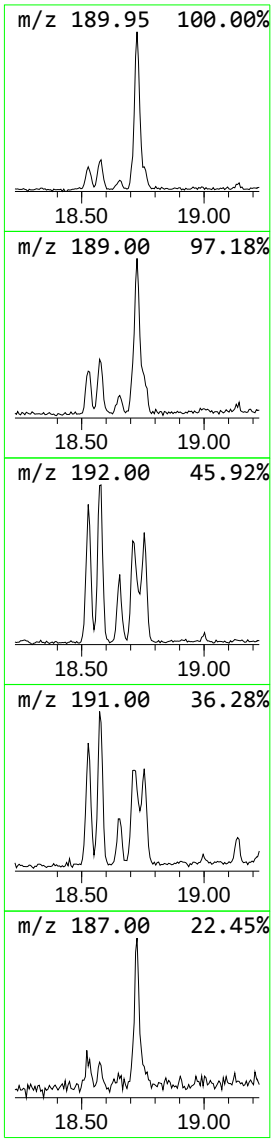
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.726	5.74 ng	178234	Phenanthrene-d10	17.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	47
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4	2-Amino-4,6-dichloropyrimidine-5...	191	C5H3Cl2N3O	005604-46-6	32
5	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	28





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Acq On : 19 Jan 2023 2:20
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Sample : 01178-01
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-011723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

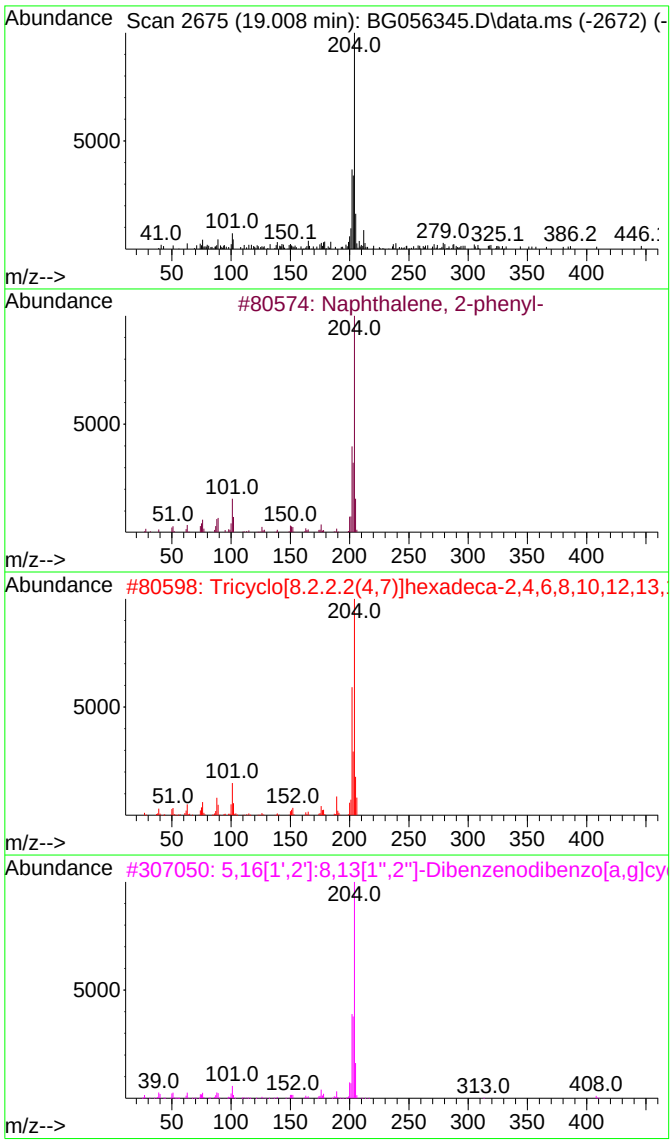
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

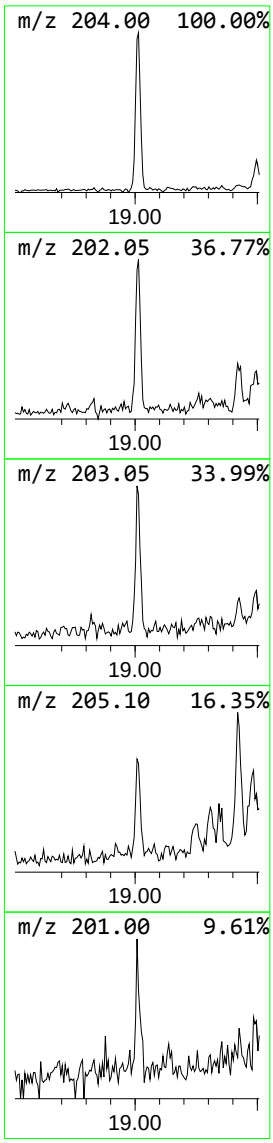
****

Peak Number 6 Naphthalene, 2-phenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.008	2.46 ng	76391	Phenanthrene-d10	17.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-phenyl-	204	C16H12	000612-94-2	76
2	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	68
3	5,16[1',2']:8,13[1'',2'']-Dibenz...	408	C32H24	005672-97-9	68
4	Acephenanthrylene, 4,5-dihydro-	204	C16H12	006232-48-0	53
5	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056345.D
Acq On : 19 Jan 2023 2:20
Operator : CG/JU
Sample : 01178-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-011723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

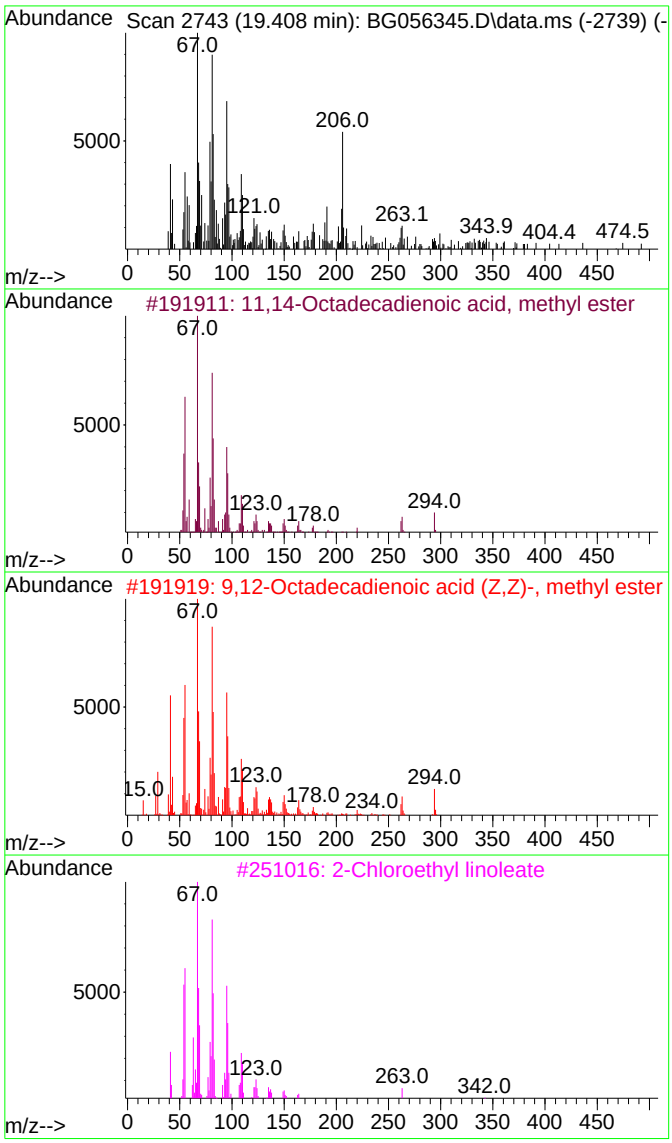
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

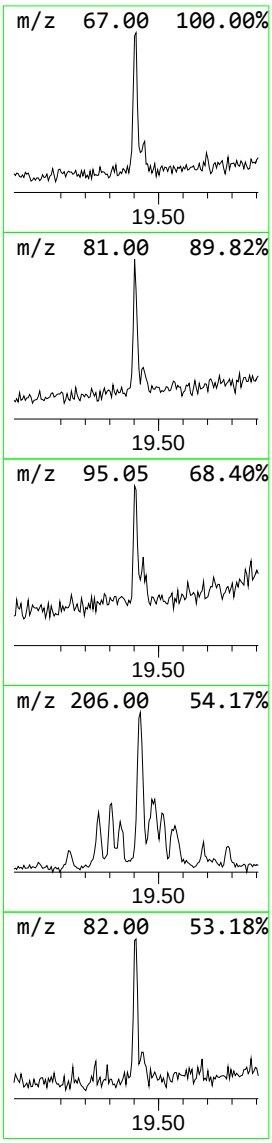
****

Peak Number 7 11,14-Octadecadienoic acid,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.408	4.21 ng	130810	Phenanthrene-d10	17.657

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	89
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	86
3	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	86
4	Linoelaidic acid	280	C18H32O2	000506-21-8	83
5	Butyl 9,12-octadecadienoate	336	C22H40O2	1000336-54-1	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056345.D
Acq On : 19 Jan 2023 2:20
Operator : CG/JU
Sample : 01178-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AU-5-011723

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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
unknown3.321	3.321	8.7	ng	108619	1	8.309	248439	20.0
2-Pentanone, 4-...	5.348	11.2	ng	139316	1	8.309	248439	20.0
Benzophenone	16.258	3.9	ng	98829	3	14.919	505484	20.0
5H-Dibenzo[a,d]...	18.573	3.3	ng	103563	4	17.657	621288	20.0
4H-Cyclopenta[d...	18.726	5.7	ng	178234	4	17.657	621288	20.0
Naphthalene, 2-...	19.008	2.5	ng	76391	4	17.657	621288	20.0
11,14-Octadecad...	19.408	4.2	ng	130810	4	17.657	621288	20.0