

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020922\
 Data File : BG052334.D
 Acq On : 9 Feb 2022 14:32
 Operator : CG/JU
 Sample : N1362-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RO-342

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-BG020722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG052334.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.828	52	58	68	rBV	143504	211840	11.81%	1.831%
2	5.755	380	386	398	rVB	428596	681132	37.97%	5.889%
3	7.376	653	662	674	rBV	448296	808132	45.05%	6.986%
4	8.228	801	807	813	rBV	103927	174034	9.70%	1.505%
5	9.397	998	1006	1014	rBV	289826	506125	28.21%	4.376%
6	11.065	1281	1290	1298	rBV	152021	271747	15.15%	2.349%
7	13.497	1696	1704	1711	rBV	766346	1199008	66.84%	10.366%
8	14.202	1817	1824	1829	rBV5	20843	30632	1.71%	0.265%
9	14.872	1932	1938	1945	rVB	271658	419865	23.40%	3.630%
10	16.358	2184	2191	2201	rBV	680483	1045445	58.28%	9.038%
11	17.621	2400	2406	2411	rBV	342071	542037	30.21%	4.686%
12	17.662	2411	2413	2419	rVB	60764	83799	4.67%	0.724%
13	18.491	2550	2554	2559	rBV2	52473	85416	4.76%	0.738%
14	18.543	2560	2563	2569	rVB	25029	40961	2.28%	0.354%
15	18.696	2583	2589	2593	rBV3	27643	55152	3.07%	0.477%
16	19.237	2677	2681	2686	rBV6	14931	27116	1.51%	0.234%
17	19.336	2693	2698	2706	rBV	685539	873949	48.72%	7.555%
18	19.407	2706	2710	2715	rVB2	25032	44824	2.50%	0.388%
19	19.665	2749	2754	2759	rVB	121638	179735	10.02%	1.554%
20	19.912	2792	2796	2801	rVB8	14321	23554	1.31%	0.204%
21	20.030	2804	2816	2823	rBV	149779	266147	14.84%	2.301%
22	20.100	2825	2828	2834	rVB8	11492	19928	1.11%	0.172%
23	20.218	2842	2848	2853	rVB	1405594	1793966	100.00%	15.509%
24	20.341	2866	2869	2872	rBV5	12087	18536	1.03%	0.160%
25	20.505	2894	2897	2905	rVB2	42196	74624	4.16%	0.645%
26	20.617	2912	2916	2920	rBV	20291	31249	1.74%	0.270%
27	20.682	2923	2927	2929	rVB2	19022	25718	1.43%	0.222%
28	20.817	2947	2950	2955	rVB2	20700	28406	1.58%	0.246%
29	21.299	3029	3032	3035	rBV2	18319	26784	1.49%	0.232%
30	21.351	3037	3041	3047	rVB	185166	263012	14.66%	2.274%
31	21.534	3068	3072	3079	rVB3	67189	108923	6.07%	0.942%
32	21.798	3112	3117	3121	rBV	105368	147121	8.20%	1.272%
33	21.939	3133	3141	3146	rBV2	307703	627229	34.96%	5.423%
34	21.986	3147	3149	3155	rVB	52251	76454	4.26%	0.661%
35	24.306	3538	3544	3552	rBV2	30891	92183	5.14%	0.797%
36	25.246	3699	3704	3713	rVB2	31688	87613	4.88%	0.757%

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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-BG020722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	25.417	3723	3733	3750	rBV3	175072	574670	32.03%	4.968%
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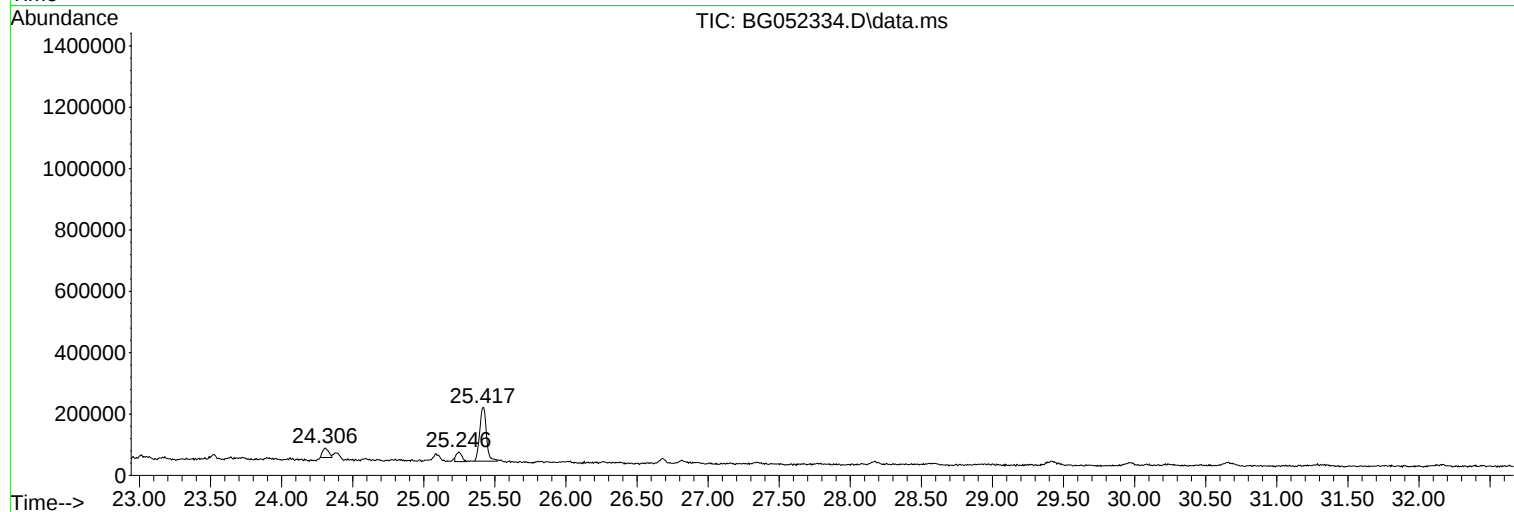
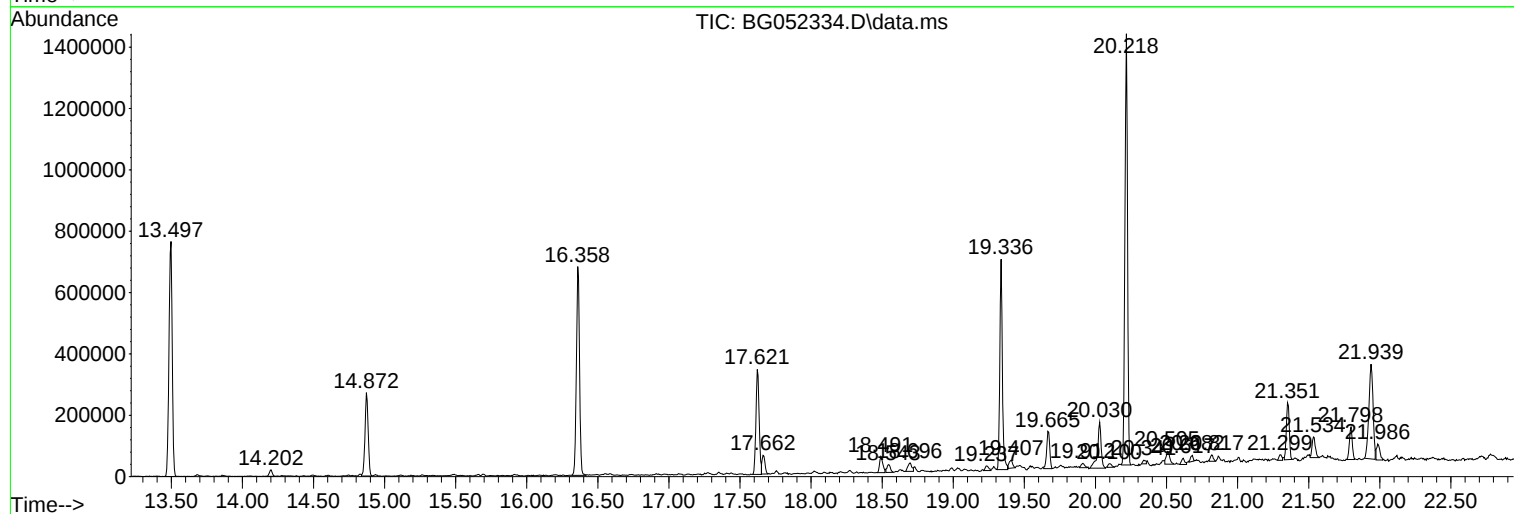
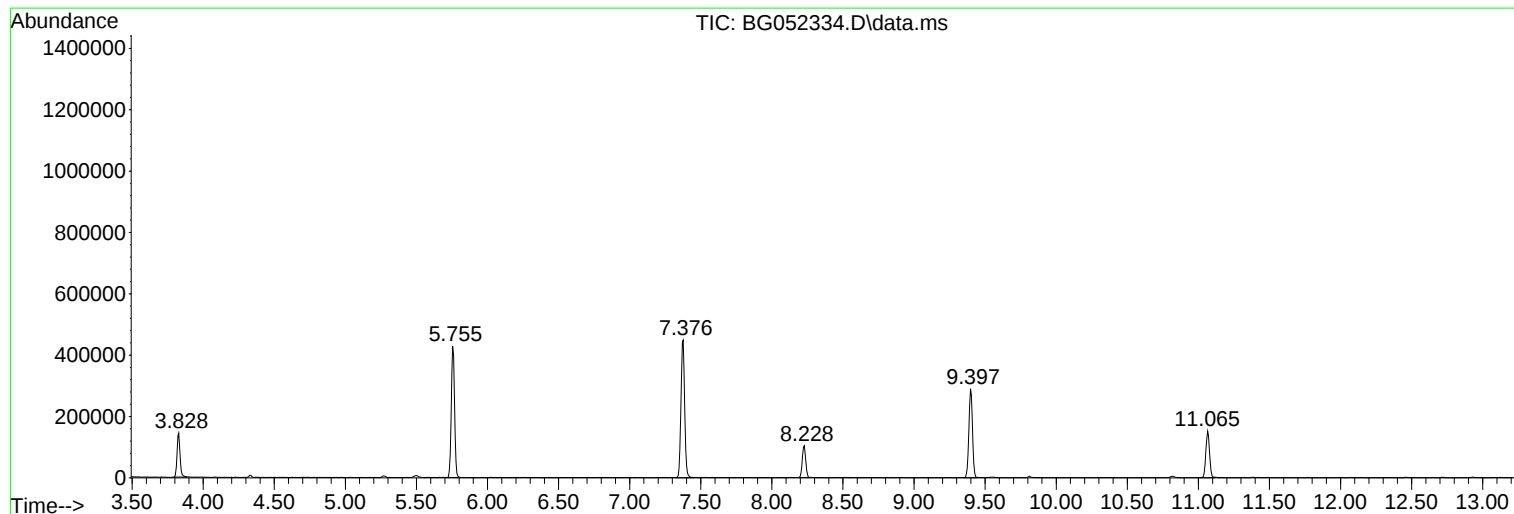
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG/JU
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ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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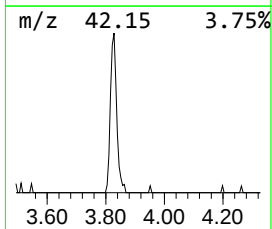
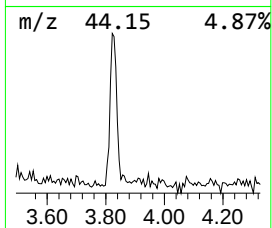
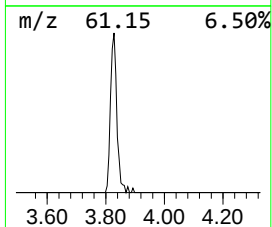
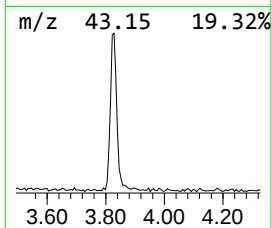
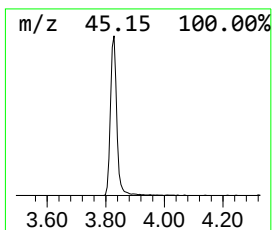
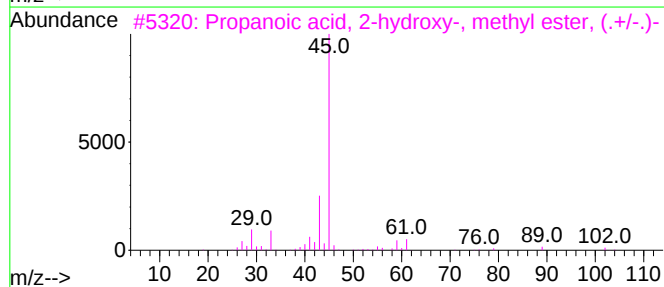
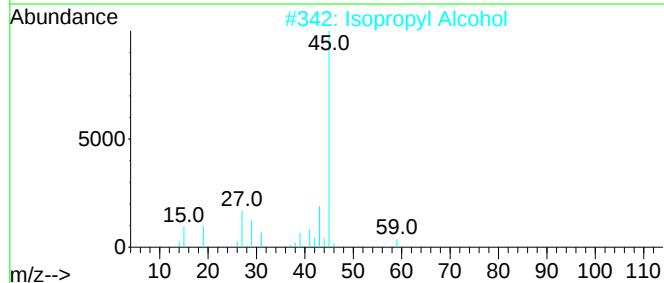
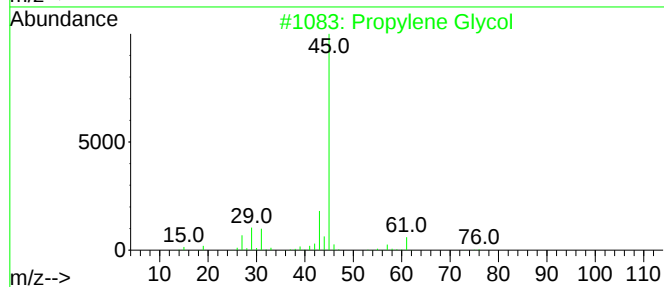
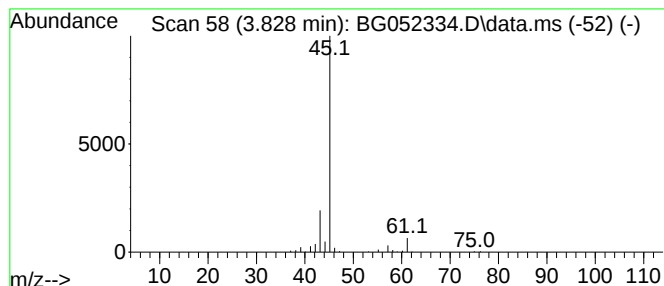
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.828	24.34 ng	211840	1,4-Dichlorobenzene-d4	8.228

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	9
5			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	7



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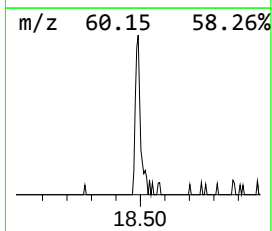
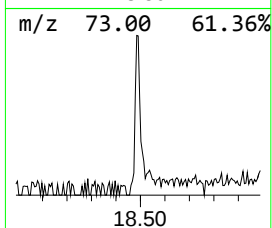
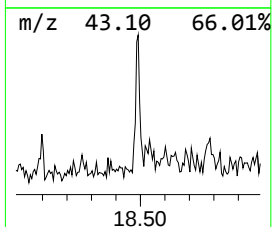
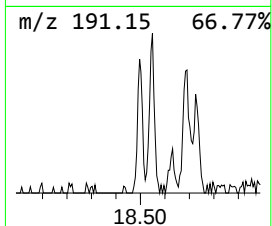
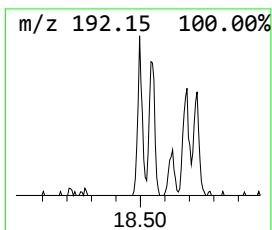
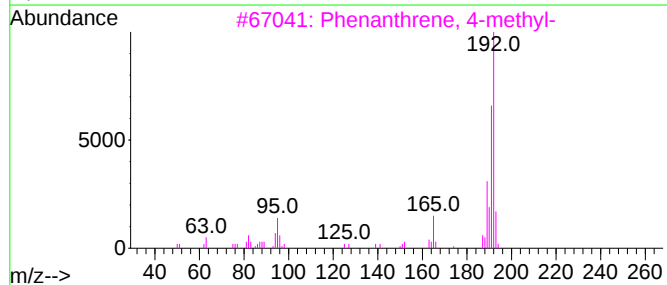
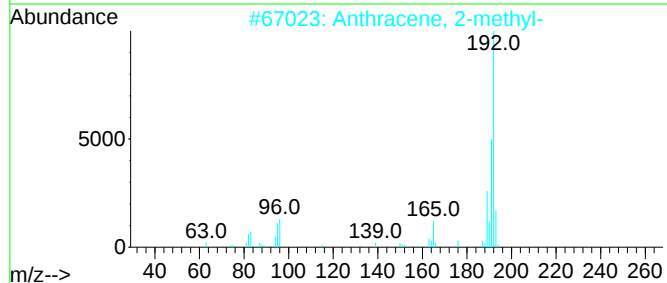
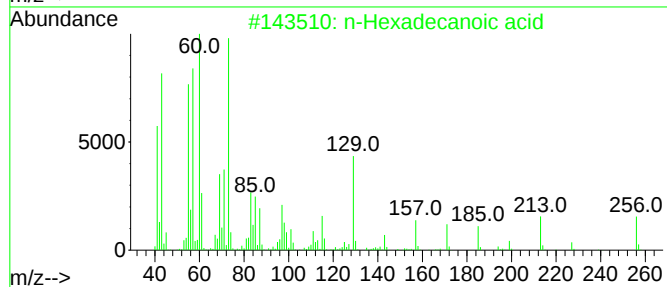
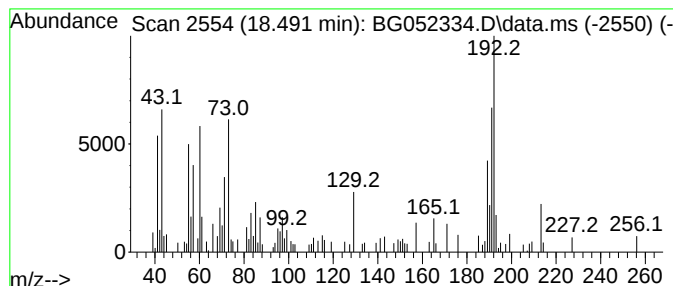
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.491	3.15 ng	85416	Phenanthrene-d10	17.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	59
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	50
3			Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	49
4			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	46
5			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	46



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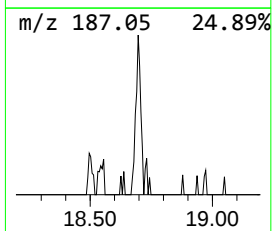
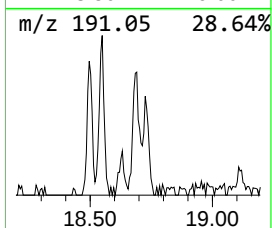
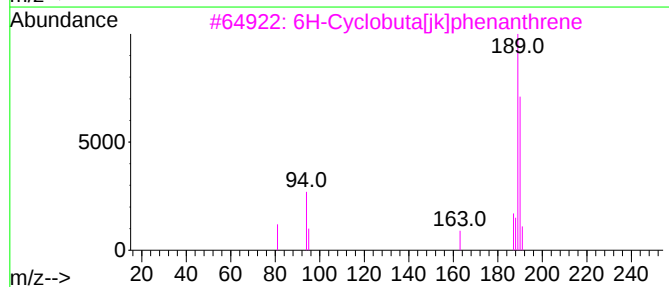
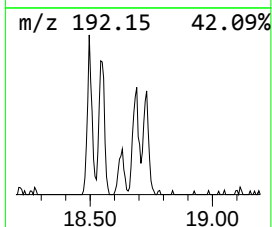
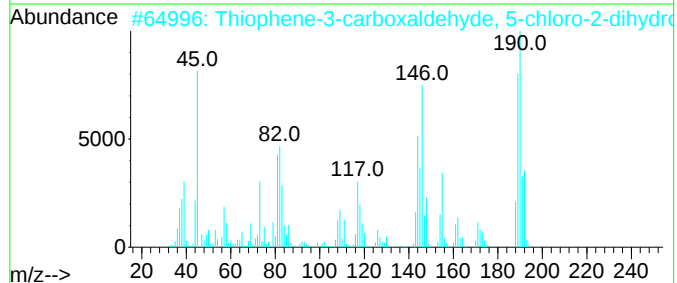
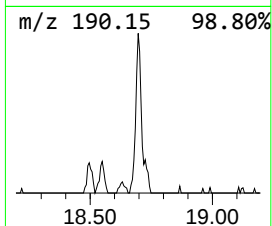
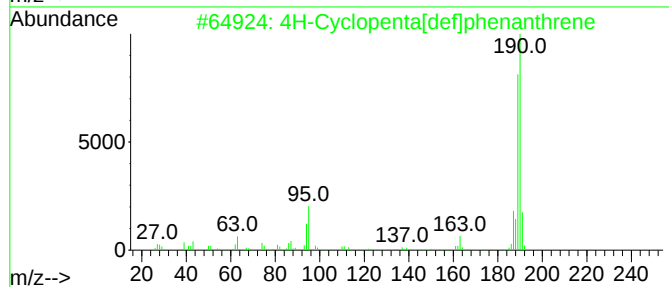
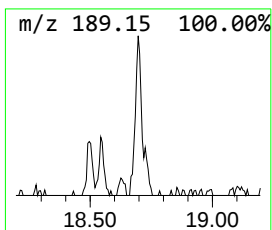
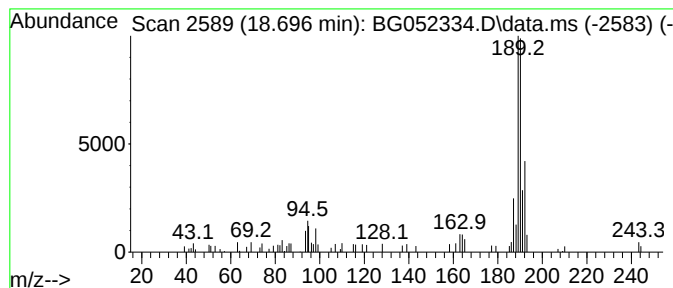
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.696	2.03 ng	55152	Phenanthrene-d10	17.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	62
2			Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	50
3			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	42
4			2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	35
5			2-Amino-4,6-dichloropyrimidine-5...	191	C5H3Cl2N3O	005604-46-6	32



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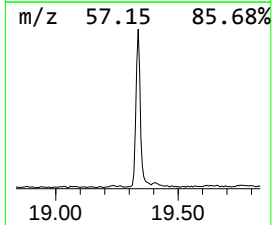
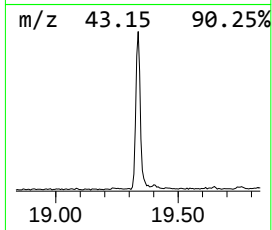
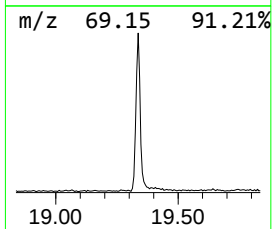
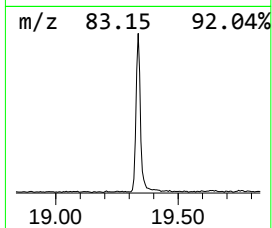
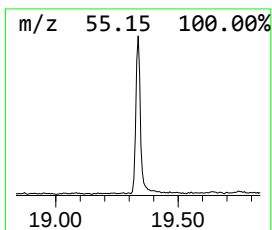
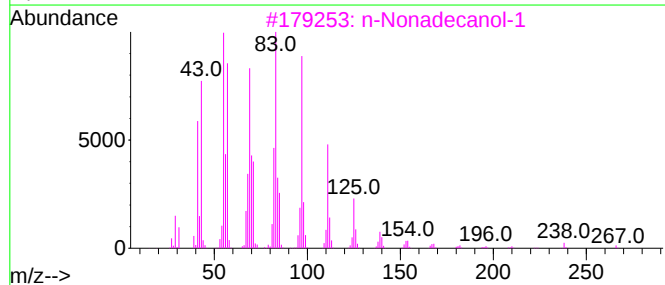
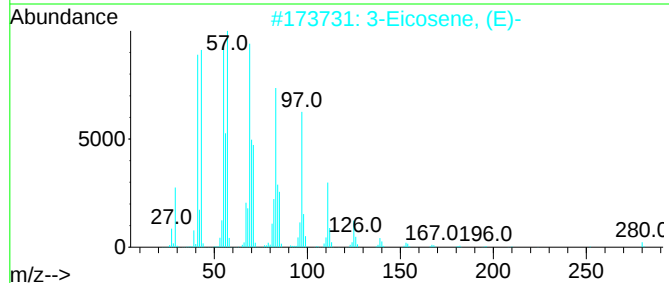
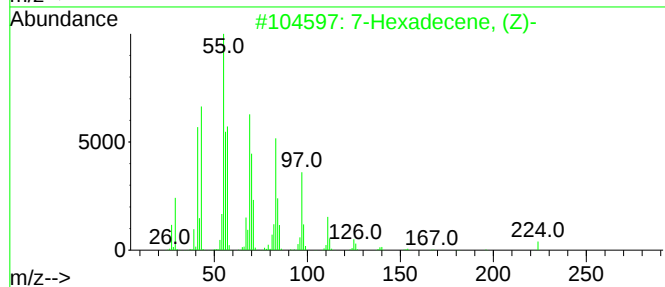
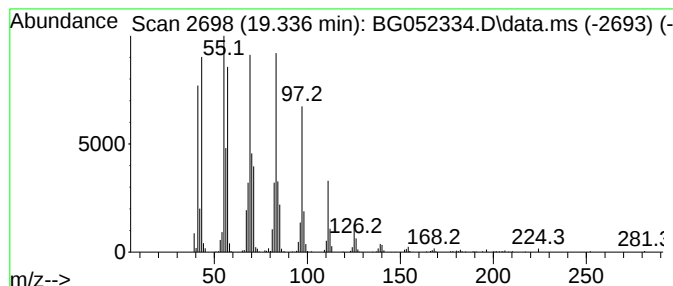
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 7-Hexadecene, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.337	32.25 ng	873949	Phenanthrene-d10		17.621	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	7-Hexadecene, (Z)-		224	C16H32	035507-09-6	97
2	3-Eicosene, (E)-		280	C20H40	074685-33-9	95
3	n-Nonadecanol-1		284	C19H40O	001454-84-8	94
4	1-Hexadecanol		242	C16H34O	036653-82-4	94
5	Trichloroacetic acid, tetradecyl...		358	C16H29Cl3O2	074339-52-9	94



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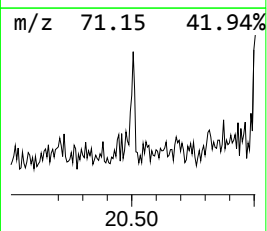
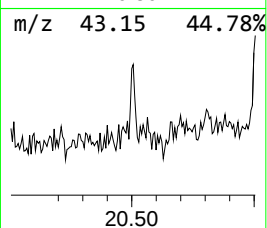
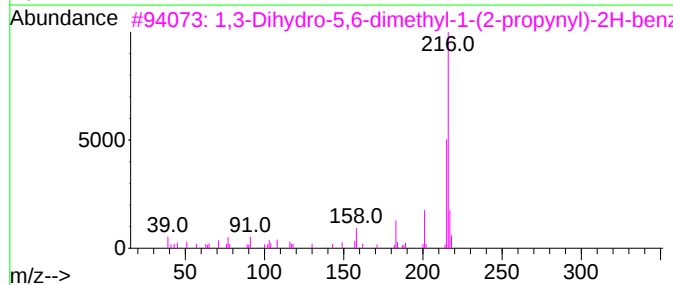
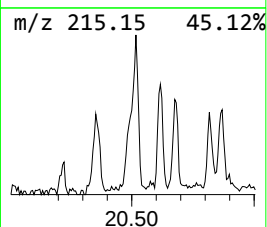
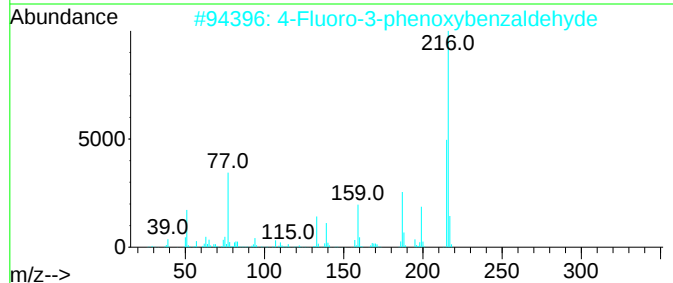
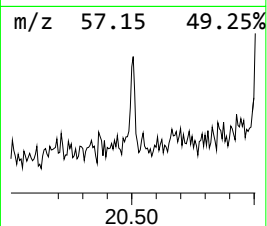
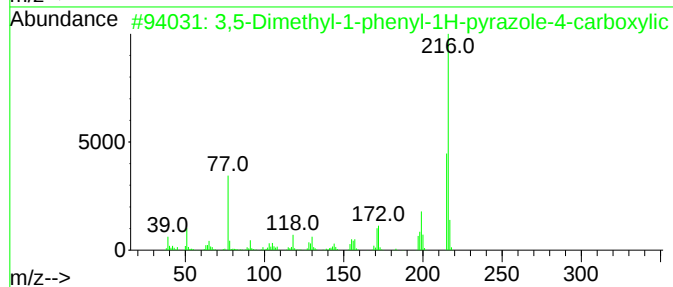
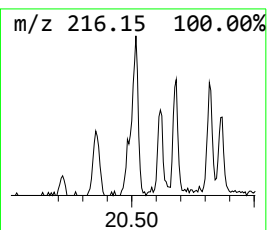
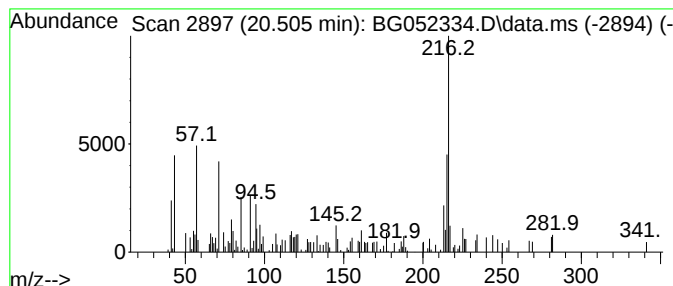
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown20.506 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.506	2.38 ng	74624	Chrysene-d12	21.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,5-Dimethyl-1-phenyl-1H-pyrazol...	216	C12H12N2O2	061226-19-5	38
2			4-Fluoro-3-phenoxybenzaldehyde	216	C13H9FO2	068359-57-9	38
3			1,3-Dihydro-5,6-dimethyl-1-(2-pr...	216	C12H12N2S	080276-22-8	38
4			5,13-Dimethyl-1,4,5,8-tetraazatr...	216	C11H12N4O	1000388-76-8	35
5			Benzoic acid, 4-(5-formyl-2-fura...	216	C12H8O4	039245-15-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020922\
Data File : BG052334.D
Acq On : 9 Feb 2022 14:32
Operator : CG/JU
Sample : N1362-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-342

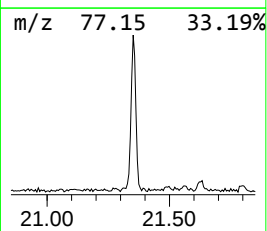
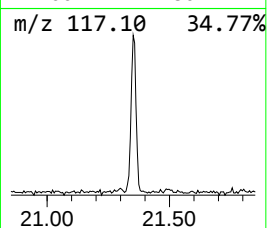
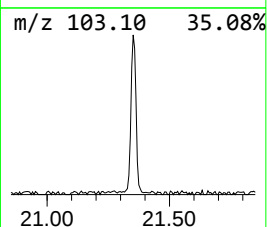
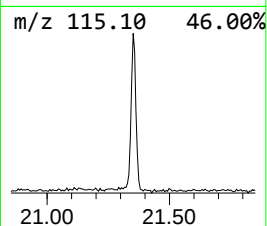
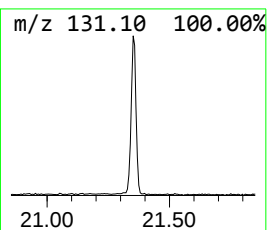
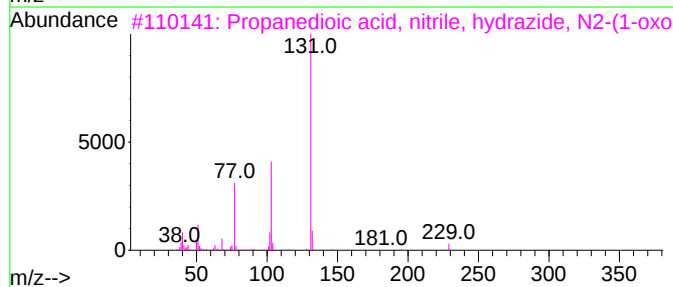
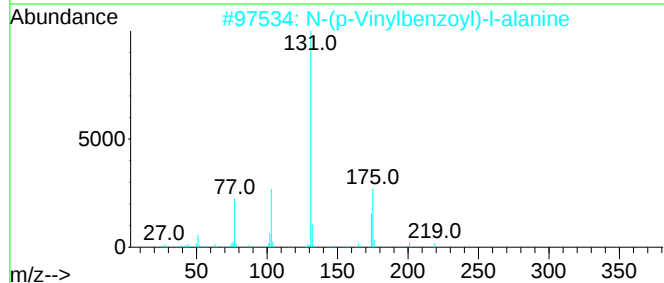
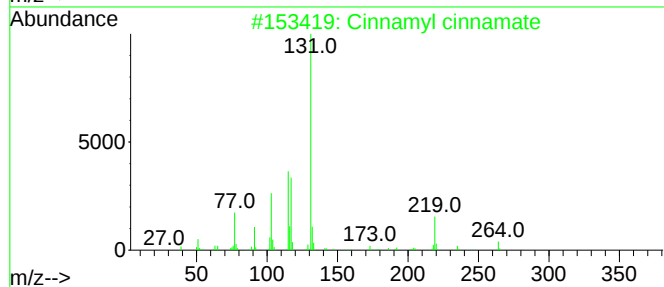
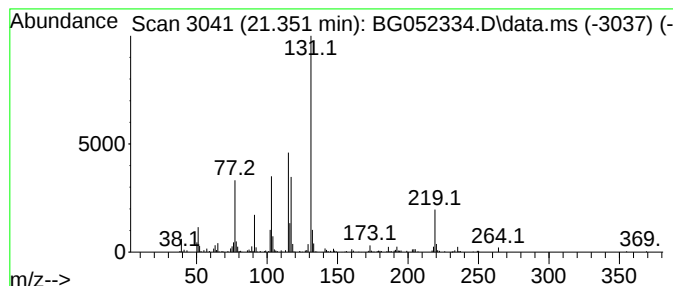
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cinnamyl cinnamate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.351	8.39 ng	263012	Chrysene-d12	21.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			N-(p-Vinylbenzoyl)-l-alanine	219	C12H13NO3	139184-60-4	47
3			Propanedioic acid, nitrile, hydr...	229	C12H11N3O2	294878-35-6	47
4			(2E)-N-(4-Methylphenyl)-3-phenyl...	237	C16H15NO	134430-88-9	47
5			N-(4-Fluorophenyl)-3-phenyl-2-pr...	241	C15H12FNO	019358-27-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020922\
Data File : BG052334.D
Acq On : 9 Feb 2022 14:32
Operator : CG/JU
Sample : N1362-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-342

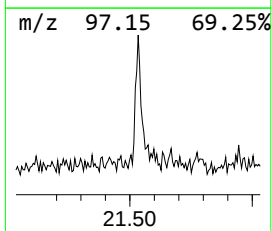
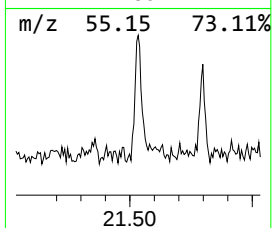
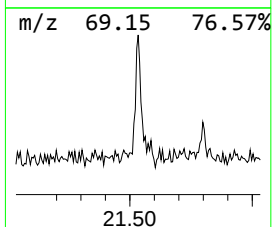
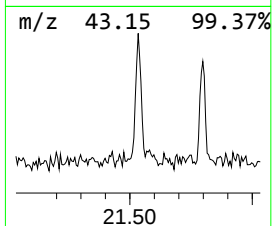
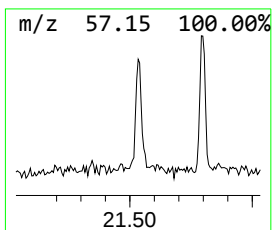
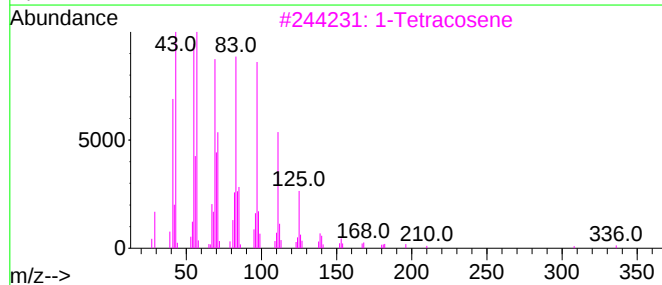
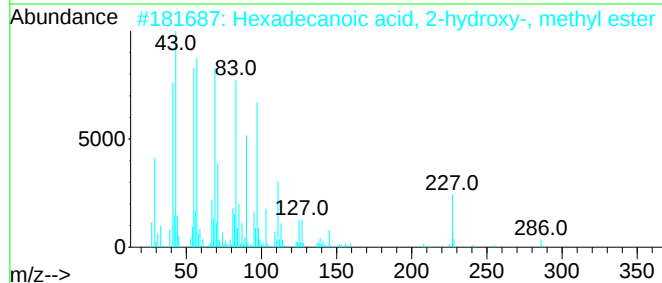
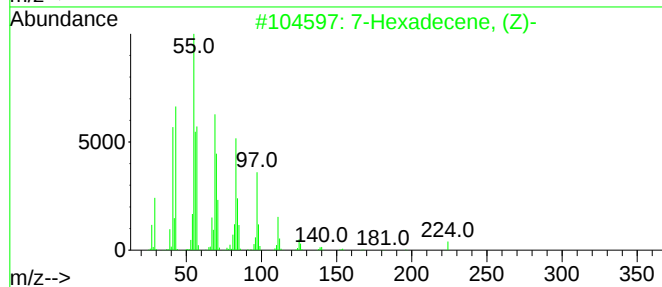
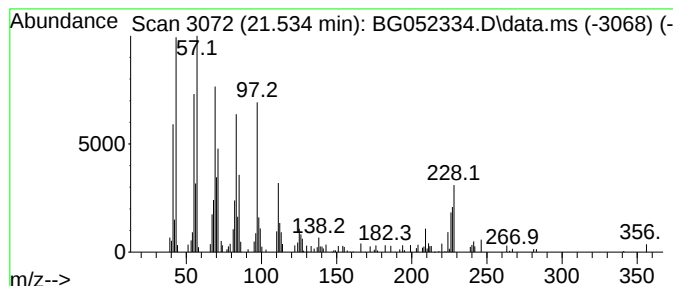
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, 2-hydrox... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.534	3.47 ng	108923	Chrysene-d12	21.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Hexadecene, (Z)-		224	C16H32		035507-09-6	89
2	Hexadecanoic acid, 2-hydroxy-, m...		286	C17H34O3		016742-51-1	64
3	1-Tetracosene		336	C24H48		010192-32-2	58
4	Cyclopentadecane		210	C15H30		000295-48-7	58
5	Trifluoroacetic acid,n-tridecyl ...		296	C15H27F3O2		053800-02-5	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG020922\
Data File : BG052334.D
Acq On : 9 Feb 2022 14:32
Operator : CG/JU
Sample : N1362-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RO-342

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propylene Glycol	3.828	24.3	ng	211840	1	8.228	174034	20.0
n-Hexadecanoic ...	18.491	3.1	ng	85416	4	17.621	542037	20.0
4H-Cyclopenta[d...]	18.696	2.0	ng	55152	4	17.621	542037	20.0
7-Hexadecene, (Z)-	19.337	32.3	ng	873949	4	17.621	542037	20.0
unknown20.506	20.506	2.4	ng	74624	5	21.939	627229	20.0
Cinnamyl cinnamate	21.351	8.4	ng	263012	5	21.939	627229	20.0
Hexadecanoic ac...	21.534	3.5	ng	108923	5	21.939	627229	20.0