

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122419\
 Data File : BP001398.D
 Acq On : 24 Dec 2019 21:04
 Operator : JU
 Sample : K6406-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 C-MUCK_12.20.19

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.605	592	598	616	rVB	189036	328671	16.10%	2.011%
2	6.211	694	701	716	rBV	1082561	1432668	70.18%	8.764%
3	7.758	956	964	977	rBV	1188530	1776569	87.03%	10.868%
4	7.928	987	993	997	rBV	1367299	1700770	83.31%	10.405%
5	8.281	1048	1053	1062	rBV	298978	336037	16.46%	2.056%
6	8.528	1088	1095	1099	rBV	1068713	1289710	63.18%	7.890%
7	9.169	1196	1204	1208	rBV	876461	1129833	55.35%	6.912%
8	10.316	1389	1399	1404	rBV	357250	423102	20.73%	2.588%
9	11.369	1569	1578	1586	rBV	37872	47956	2.35%	0.293%
10	12.098	1694	1702	1706	rBV	1644581	1964048	96.21%	12.015%
11	12.298	1731	1736	1741	rVB	18377	21459	1.05%	0.131%
12	12.763	1810	1815	1820	rBV	69526	76660	3.76%	0.469%
13	13.175	1879	1885	1894	rBV	416190	525900	25.76%	3.217%
14	14.475	2098	2106	2120	rBV	1176995	1476181	72.31%	9.031%
15	15.575	2283	2293	2298	rBV	475710	564468	27.65%	3.453%
16	15.716	2313	2317	2322	rVB2	24584	26824	1.31%	0.164%
17	16.469	2439	2445	2452	rBV2	45050	65230	3.20%	0.399%
18	17.869	2676	2683	2686	rBV	1817955	2041401	100.00%	12.488%
19	19.104	2888	2893	2902	rBV2	44493	73674	3.61%	0.451%
20	19.222	2908	2913	2918	rVB	416347	442421	21.67%	2.707%
21	19.510	2959	2962	2971	rVB	23279	27643	1.35%	0.169%
22	19.904	3023	3029	3033	rBV	22167	29279	1.43%	0.179%
23	20.275	3089	3092	3096	rVB	26068	30605	1.50%	0.187%
24	20.669	3155	3159	3164	rBV	29634	38150	1.87%	0.233%
25	20.992	3208	3214	3220	rVB	280351	380465	18.64%	2.328%
26	21.104	3228	3233	3239	rVB	27006	38765	1.90%	0.237%
27	21.592	3312	3316	3322	rVB2	19044	30606	1.50%	0.187%
28	22.163	3407	3413	3421	rVB3	12626	27320	1.34%	0.167%

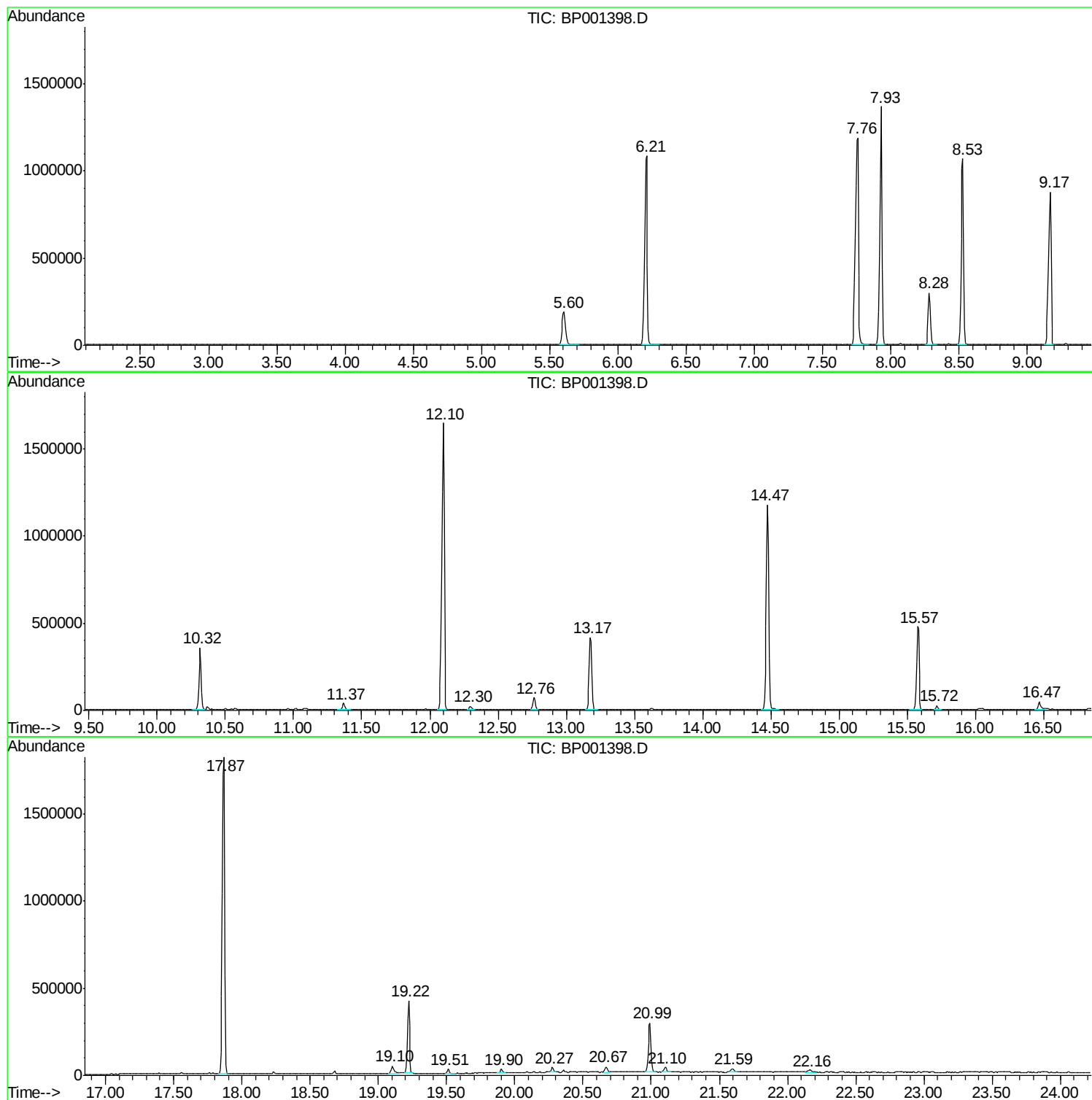
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP121919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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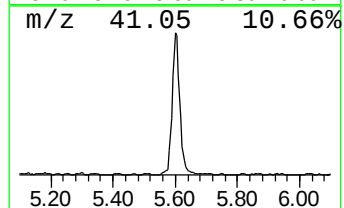
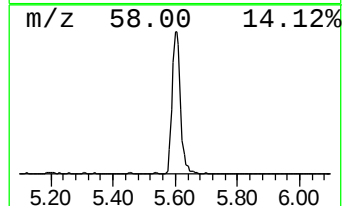
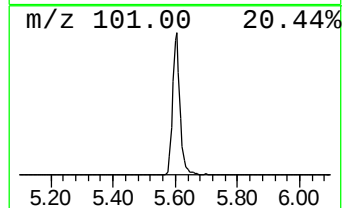
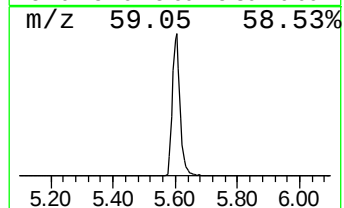
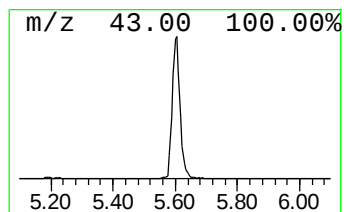
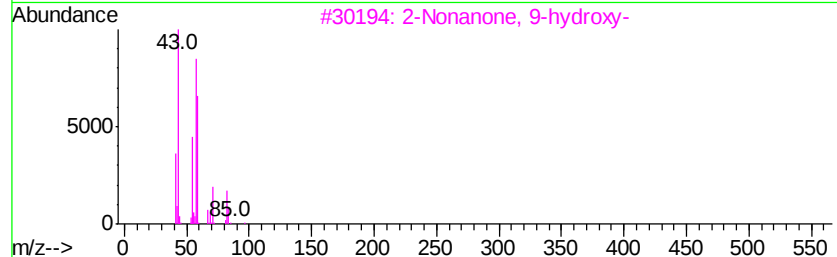
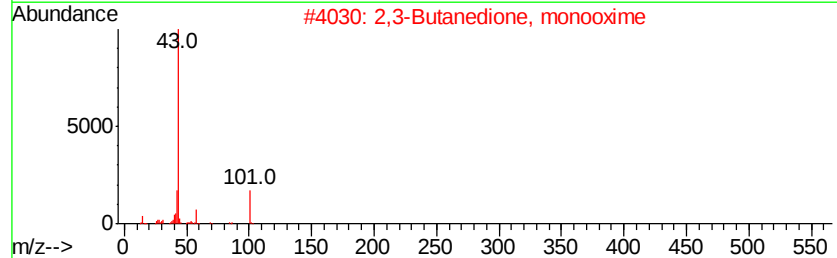
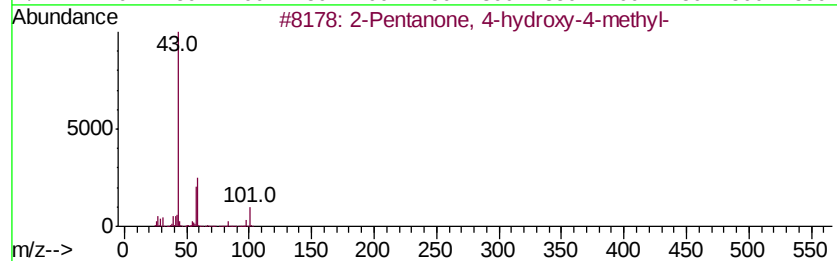
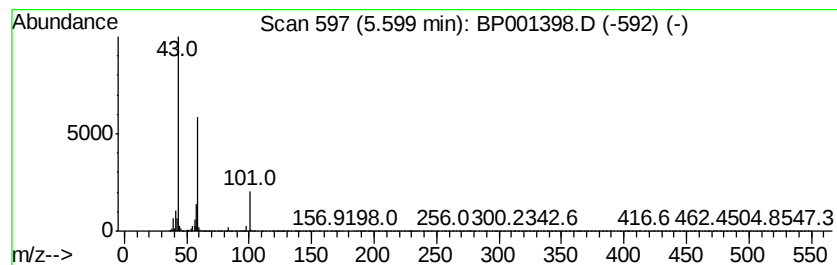
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	19.56 ng	328671	1,4-Dichlorobenzene-d4	8.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane	58	C4H10	000106-97-8	9



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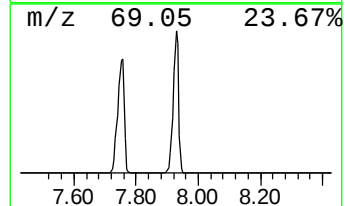
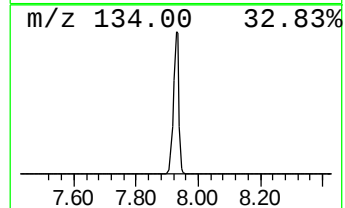
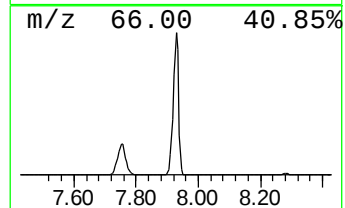
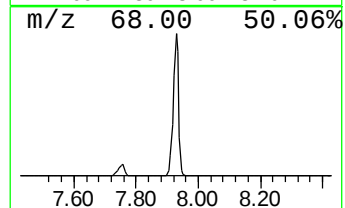
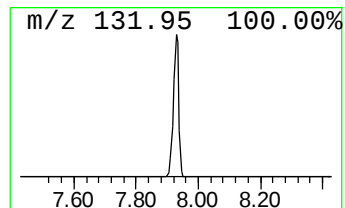
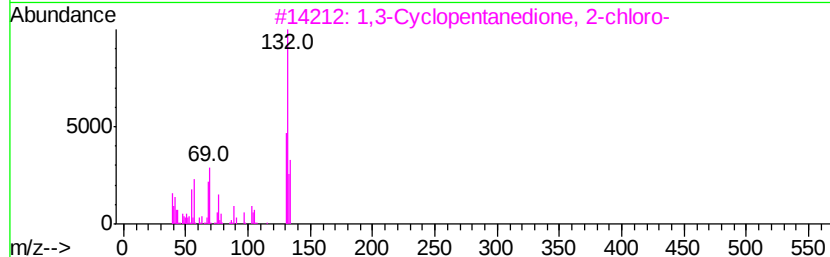
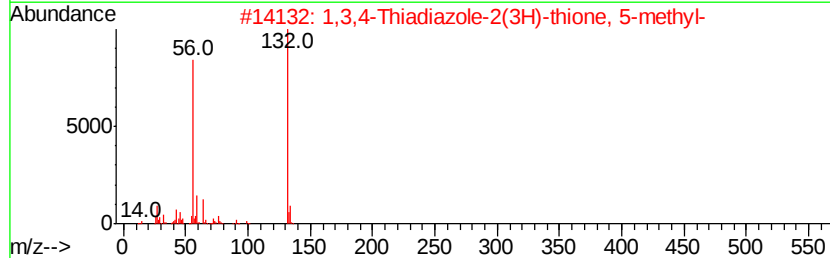
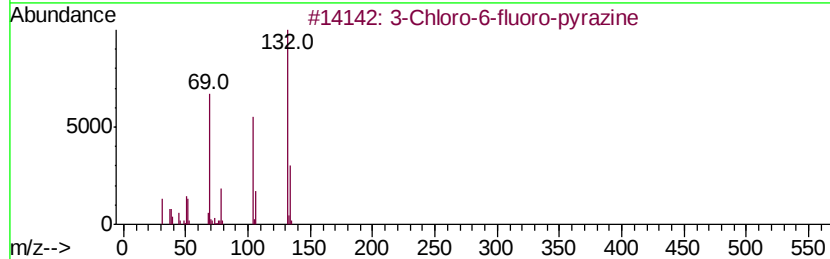
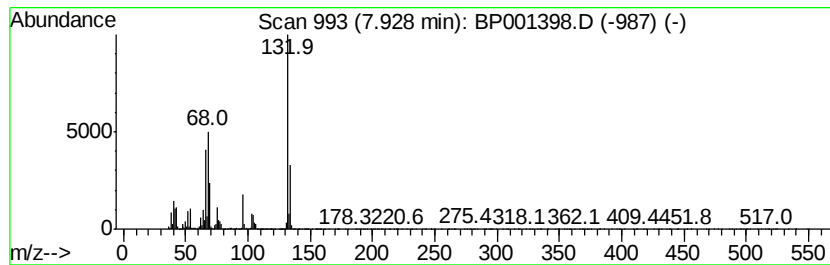
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Peak Number 2 unknown7.93 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.93	101.23 ng	1700770	1,4-Dichlorobenzene-d4	8.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
4		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	10
5		5-Aminoindole	132	C8H8N2	005192-03-0	10



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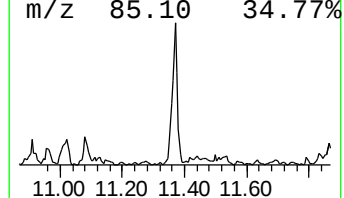
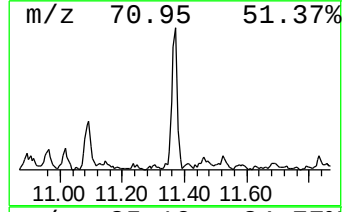
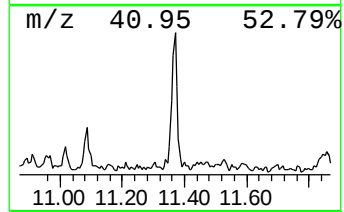
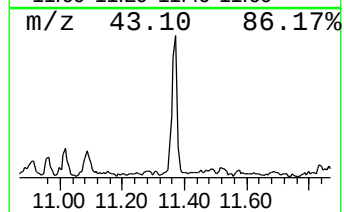
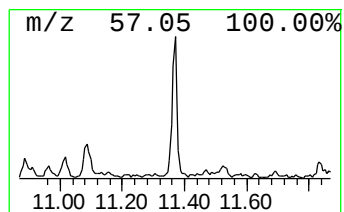
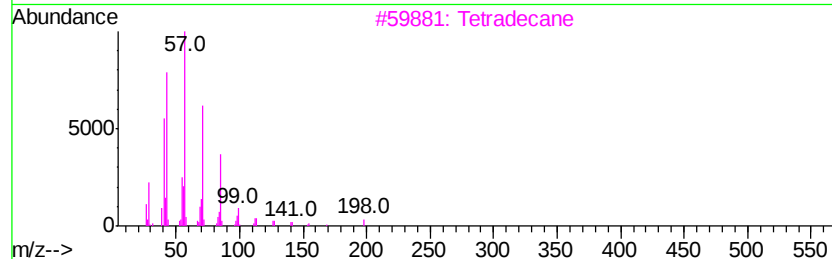
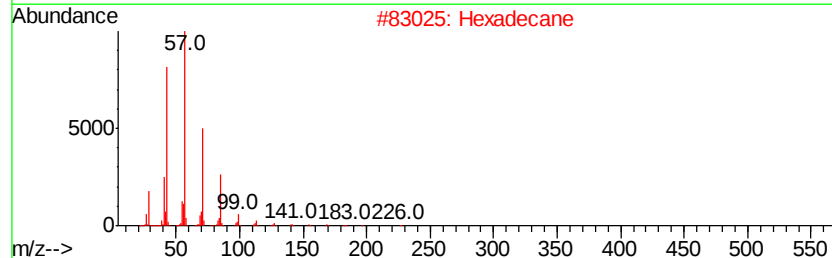
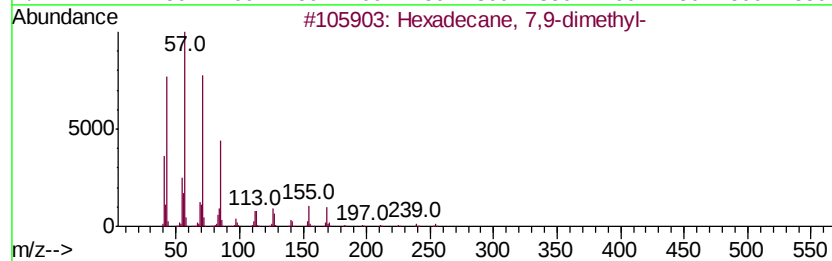
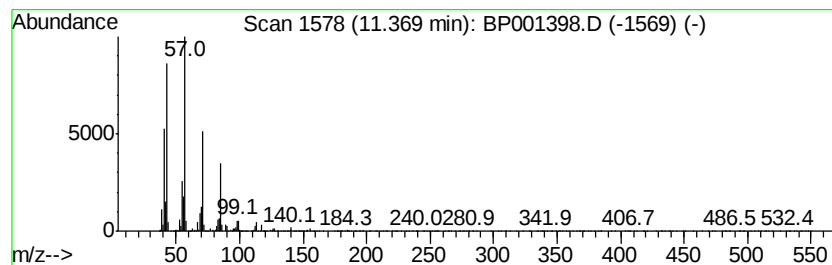
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane, 7,9-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.37	2.27 ng	47956	Naphthalene-d8	10.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	90
2		Hexadecane	226	C16H34	000544-76-3	90
3		Tetradecane	198	C14H30	000629-59-4	90
4		Pentadecane	212	C15H32	000629-62-9	87
5		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83



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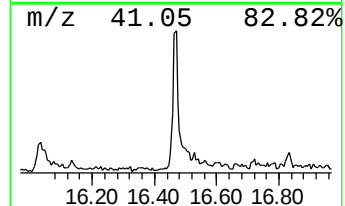
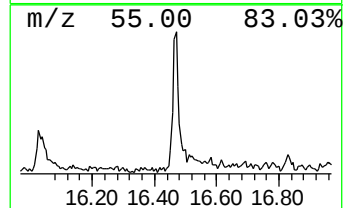
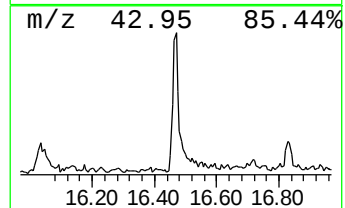
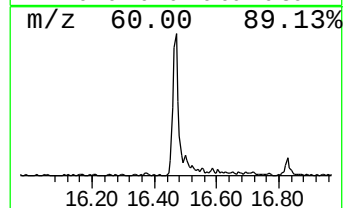
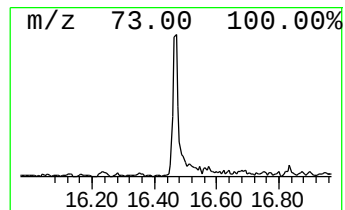
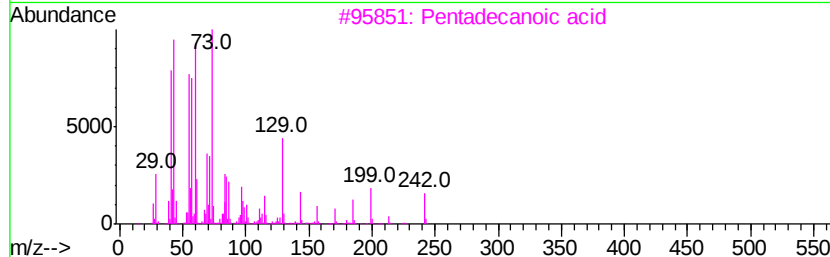
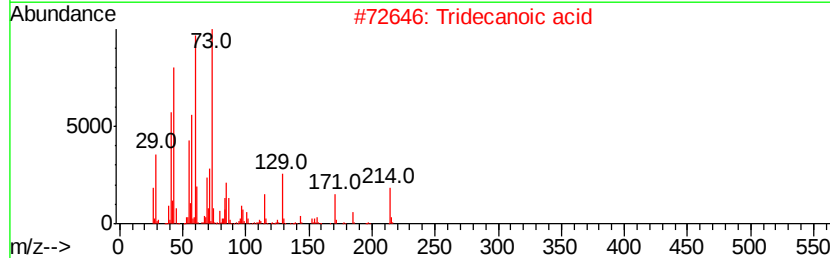
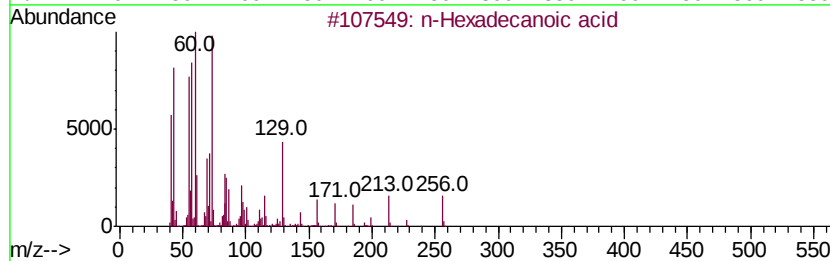
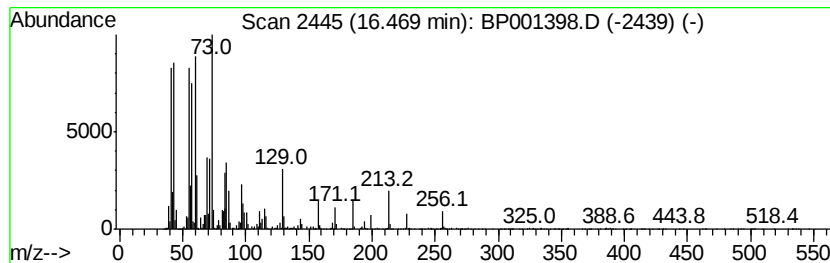
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.47	2.31 ng	65230	Phenanthrene-d10	15.57

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	81
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4		Dodecanoic acid	200	C12H24O2	000143-07-7	74
5		Octadecanoic acid	284	C18H36O2	000057-11-4	74



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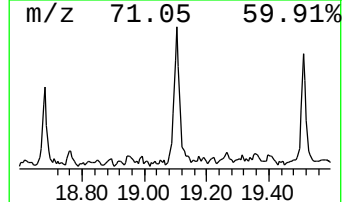
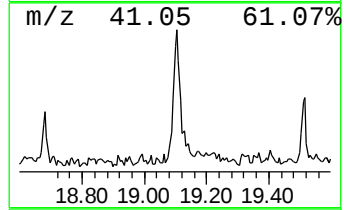
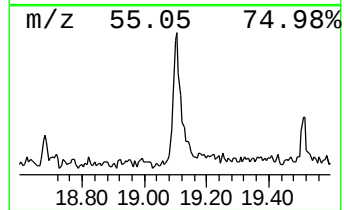
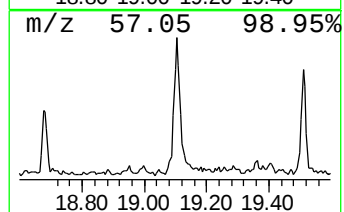
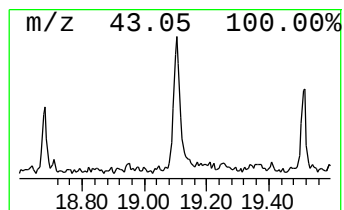
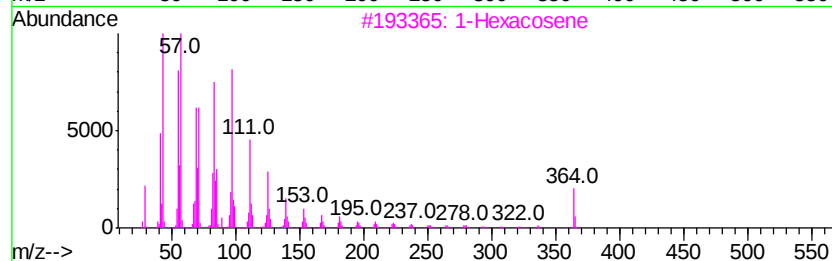
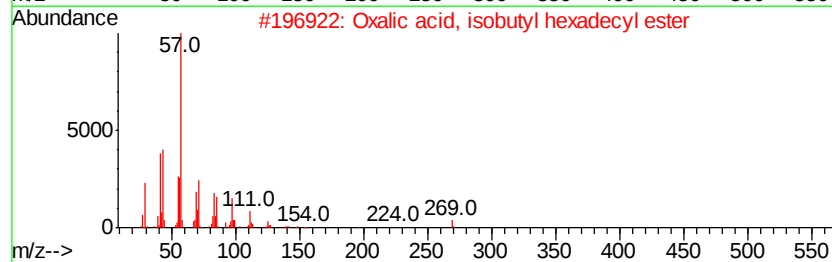
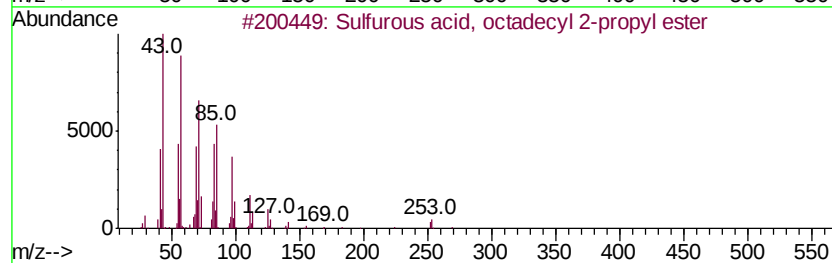
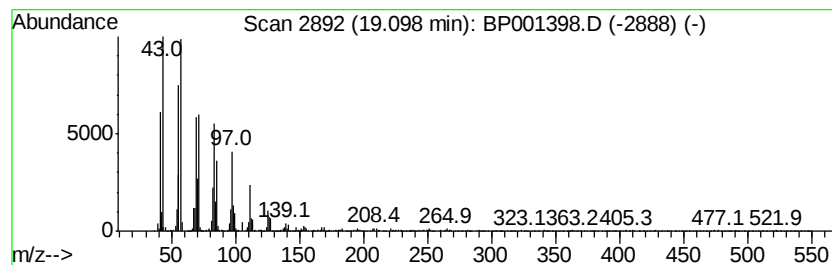
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TIC Library : C:\DATABASE\NIST11.L
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 Peak Number 6 Sulfurous acid, octadecyl 2... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.10	3.33 ng	73674	Chrysene-d12	19.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	80
2		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	74
3		1-Hexacosene	364	C26H52	018835-33-1	70
4		2-Octyldodecyl butyrate	368	C24H48O2	1000368-55-2	70
5		1-Octadecene	252	C18H36	000112-88-9	70



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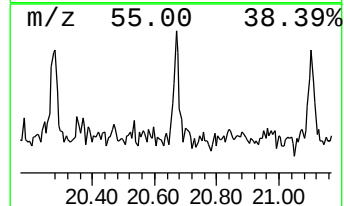
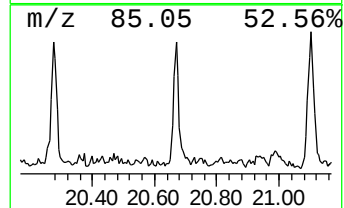
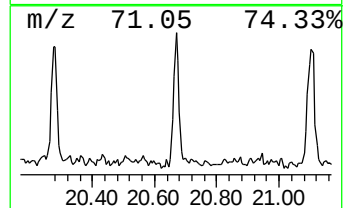
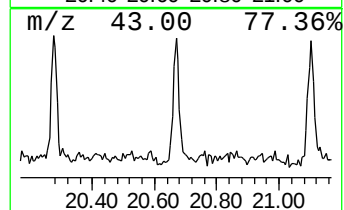
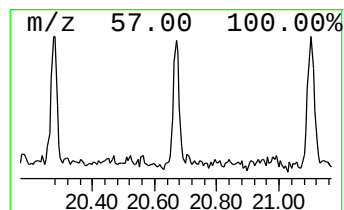
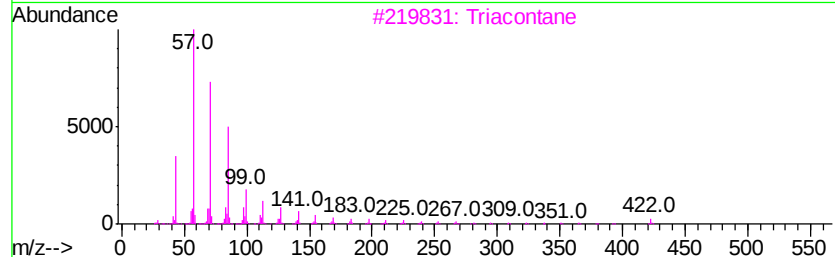
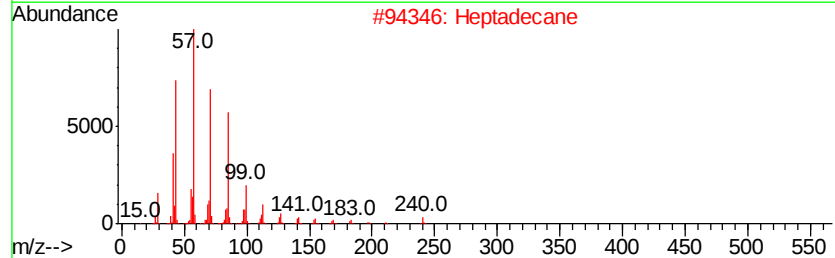
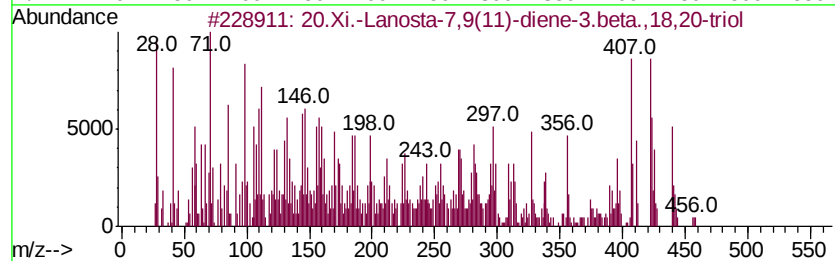
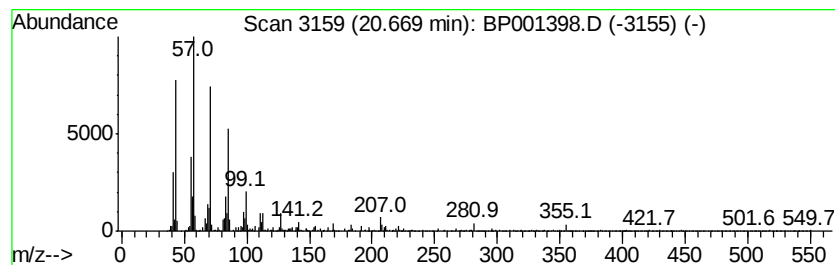
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 20.Xi.-Lanosta-7,9(11)-dien... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.67	2.01 ng	38150	Perylene-d12	20.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	20.Xi.-Lanosta-7,9(11)-diene-3.b...	458	C30H50O3	025116-58-9	97
2		Heptadecane	240	C17H36	000629-78-7	87
3		Triacontane	422	C30H62	000638-68-6	83
4		Docosane	310	C22H46	000629-97-0	83
5		Hexadecane	226	C16H34	000544-76-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122419\
Data File : BP001398.D
Acq On : 24 Dec 2019 21:04
Operator : JU
Sample : K6406-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C-MUCK_12.20.19

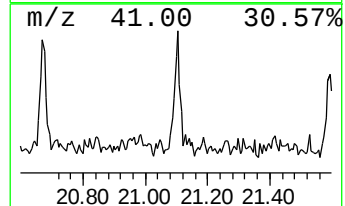
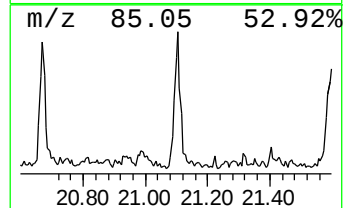
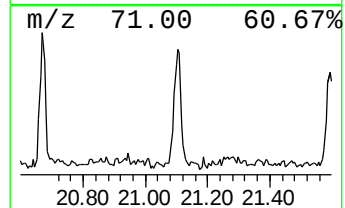
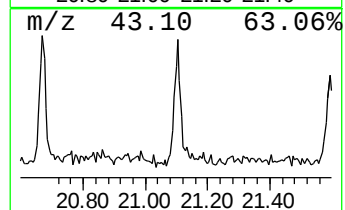
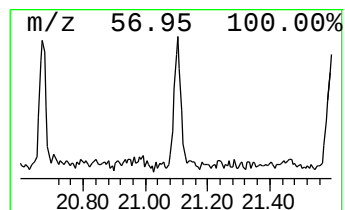
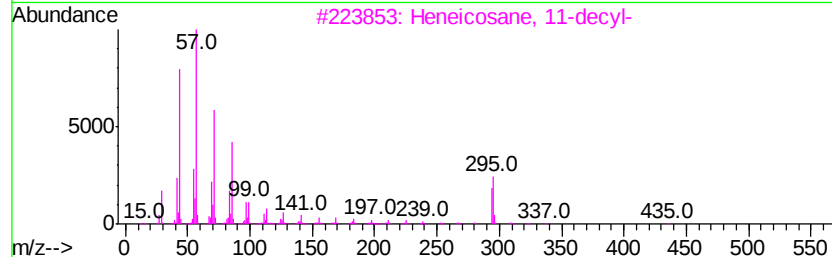
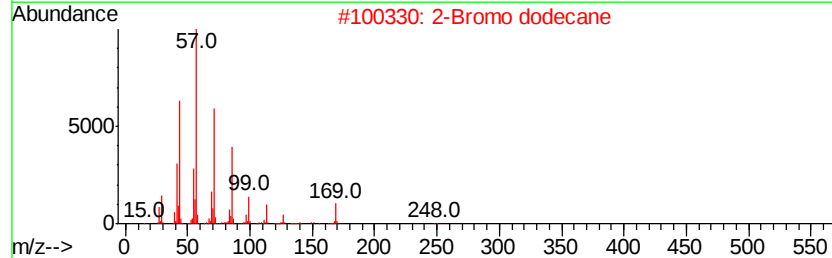
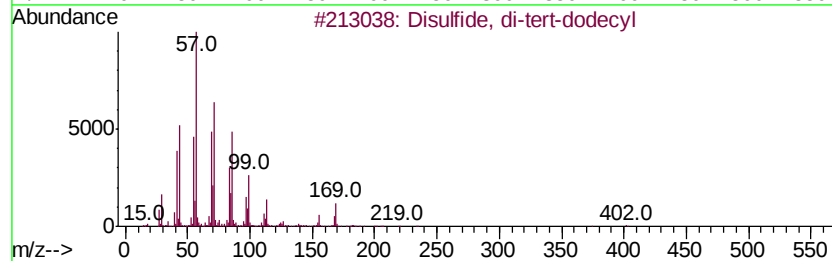
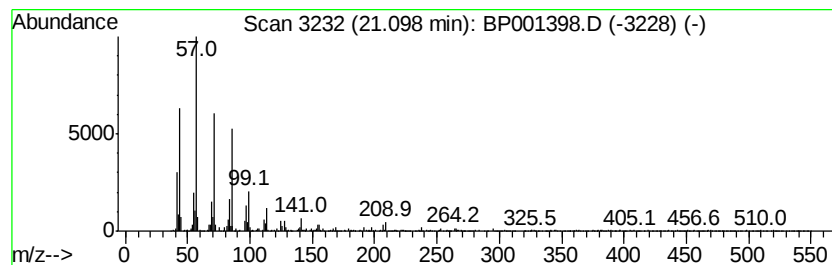
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Disulfide, di-tert-dodecyl Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.10	2.04 ng	38765	Perylene-d12	20.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	90
2		2-Bromo dodecane	248	C12H25Br	013187-99-0	90
3		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	83
4		Tetratetracontane	619	C44H90	007098-22-8	68
5		Octacosane	394	C28H58	000630-02-4	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP122419\
Data File : BP001398.D
Acq On : 24 Dec 2019 21:04
Operator : JU
Sample : K6406-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C-MUCK_12.20.19

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.60	19.6	ng	328671	1	8.28	336037	20.0
unknown7.93	7.93	101.2	ng	1700770	1	8.28	336037	20.0
Hexadecane, 7,9-d...	11.37	2.3	ng	47956	2	10.32	423102	20.0
n-Hexadecanoic acid	16.47	2.3	ng	65230	4	15.57	564468	20.0
Sulfurous acid, o...	19.10	3.3	ng	73674	5	19.22	442421	20.0
20.Xi.-Lanosta-7,...	20.67	2.0	ng	38150	6	20.99	380465	20.0
Disulfide, di-ter...	21.10	2.0	ng	38765	6	20.99	380465	20.0