

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
 Data File : BF124210.D
 Acq On : 9 Jun 2021 15:49
 Operator : JU/CG
 Sample : M2598-10
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 17

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-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124210.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.346	206	214	228	rBV	39650	102361	18.49%	1.943%
2	5.469	572	575	582	rBV	448628	423451	76.49%	8.038%
3	6.487	744	748	757	rBV	506798	429679	77.62%	8.156%
4	6.846	806	809	812	rBV	294117	213239	38.52%	4.048%
5	7.404	900	904	907	rBV	362293	298328	53.89%	5.663%
6	8.128	1024	1027	1031	rBV	347306	266266	48.10%	5.054%
7	8.228	1041	1044	1048	rBV2	7906	8297	1.50%	0.157%
8	9.204	1206	1210	1213	rBV	762565	553588	100.00%	10.508%
9	9.357	1233	1236	1246	rBV	49305	67779	12.24%	1.287%
10	9.886	1322	1326	1329	rVB	413937	327469	59.15%	6.216%
11	10.669	1456	1459	1466	rBV	398320	363973	65.75%	6.909%
12	10.786	1476	1479	1484	rBV2	8611	12294	2.22%	0.233%
13	10.981	1506	1512	1515	rBV2	4383	7328	1.32%	0.139%
14	11.233	1552	1555	1557	rVB	13458	10202	1.84%	0.194%
15	11.369	1575	1578	1581	rBV	364896	305520	55.19%	5.799%
16	11.392	1581	1582	1585	rVB	37992	23326	4.21%	0.443%
17	11.657	1625	1627	1632	rBV3	6578	8287	1.50%	0.157%
18	11.898	1665	1668	1671	rVB2	23333	22804	4.12%	0.433%
19	12.069	1693	1697	1699	rBV3	7286	9136	1.65%	0.173%
20	12.198	1715	1719	1721	rBV3	6282	9316	1.68%	0.177%
21	12.457	1759	1763	1766	rBV4	11012	10176	1.84%	0.193%
22	12.586	1779	1785	1789	rBV	48835	49964	9.03%	0.948%
23	12.680	1798	1801	1804	rBV3	7928	8262	1.49%	0.157%
24	12.816	1818	1824	1828	rBV	39370	50243	9.08%	0.954%
25	12.863	1828	1832	1837	rVB7	7897	12421	2.24%	0.236%
26	12.951	1844	1847	1851	rBV	469096	435702	78.71%	8.270%
27	13.139	1877	1879	1884	rVB6	11016	12483	2.25%	0.237%
28	13.180	1884	1886	1888	rBV3	8152	7580	1.37%	0.144%
29	13.310	1904	1908	1909	rBV4	9588	9702	1.75%	0.184%
30	13.433	1926	1929	1937	rBV8	11554	28019	5.06%	0.532%
31	13.527	1940	1945	1946	rBV5	10631	11200	2.02%	0.213%
32	13.639	1960	1964	1965	rBV4	11077	15012	2.71%	0.285%
33	13.739	1979	1981	1983	rBV3	8298	8512	1.54%	0.162%
34	13.763	1983	1985	1988	rVB3	11139	10476	1.89%	0.199%
35	13.792	1988	1990	1991	rBV2	9172	8056	1.46%	0.153%
36	13.874	1997	2004	2010	rVB8	25720	54682	9.88%	1.038%

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37	14.010	2020	2027	2031	rBV	286021	327420	59.15%	6.215%
38	14.039	2031	2032	2034	rVB2	22069	9045	1.63%	0.172%
39	14.174	2052	2055	2058	rBV5	9617	14075	2.54%	0.267%
40	14.392	2091	2092	2096	rBV4	10341	13347	2.41%	0.253%
41	14.786	2156	2159	2161	rBV4	22996	21030	3.80%	0.399%
42	15.010	2194	2197	2200	rBV5	15682	19307	3.49%	0.366%
43	15.057	2201	2205	2212	rVV6	31043	72532	13.10%	1.377%
44	15.127	2214	2217	2222	rVB4	34314	42412	7.66%	0.805%
45	15.486	2274	2278	2288	rVB2	223140	317637	57.38%	6.029%
46	15.945	2353	2356	2360	rVB4	31113	42940	7.76%	0.815%
47	16.345	2423	2424	2426	rBV2	10241	9100	1.64%	0.173%
48	16.627	2469	2472	2477	rBV6	19018	33224	6.00%	0.631%
49	17.039	2539	2542	2544	rBV4	17027	22807	4.12%	0.433%
50	17.145	2558	2560	2562	rBV3	11178	10135	1.83%	0.192%
51	17.180	2564	2566	2567	rBV2	13126	8981	1.62%	0.170%
52	17.204	2567	2570	2577	rVV9	16681	32302	5.84%	0.613%
53	17.280	2581	2583	2587	rVB5	14501	14155	2.56%	0.269%
54	17.345	2592	2594	2596	rBV3	9936	7558	1.37%	0.143%
55	17.492	2617	2619	2621	rBV3	10822	9235	1.67%	0.175%
56	17.715	2655	2657	2658	rBV2	9993	9179	1.66%	0.174%
57	17.839	2676	2678	2679	rBV2	13351	7432	1.34%	0.141%
58	18.015	2707	2708	2711	rBV3	12868	13478	2.43%	0.256%
59	18.062	2715	2716	2718	rBV2	7961	7443	1.34%	0.141%
60	18.409	2773	2775	2778	rBV4	9191	8420	1.52%	0.160%

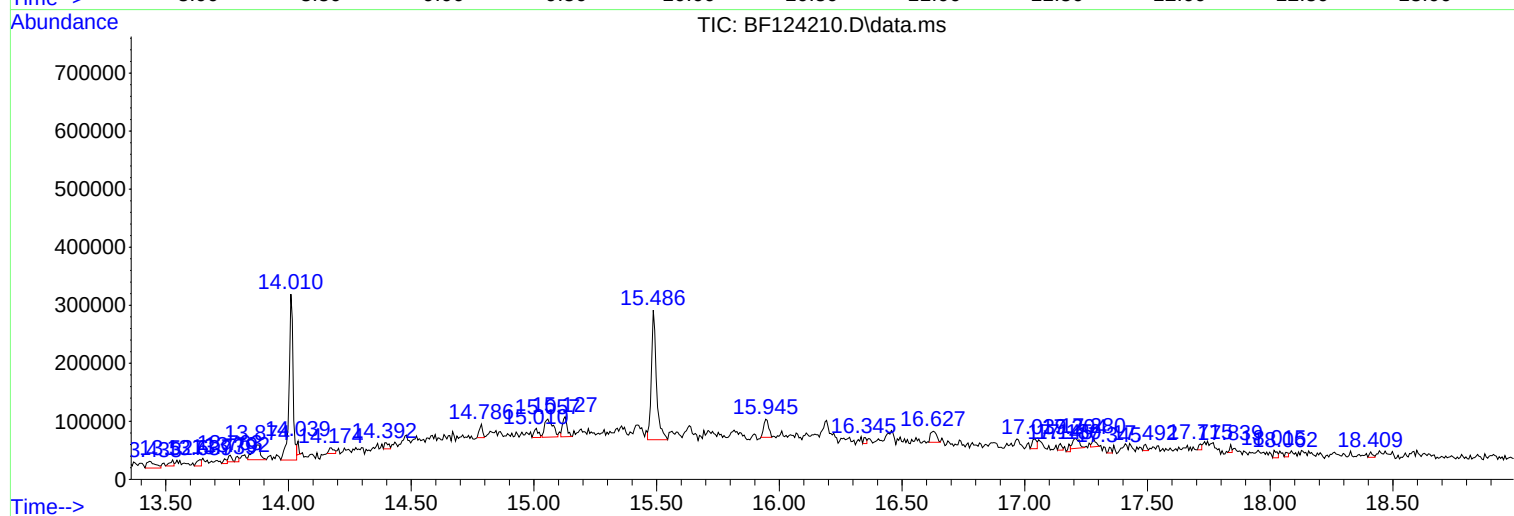
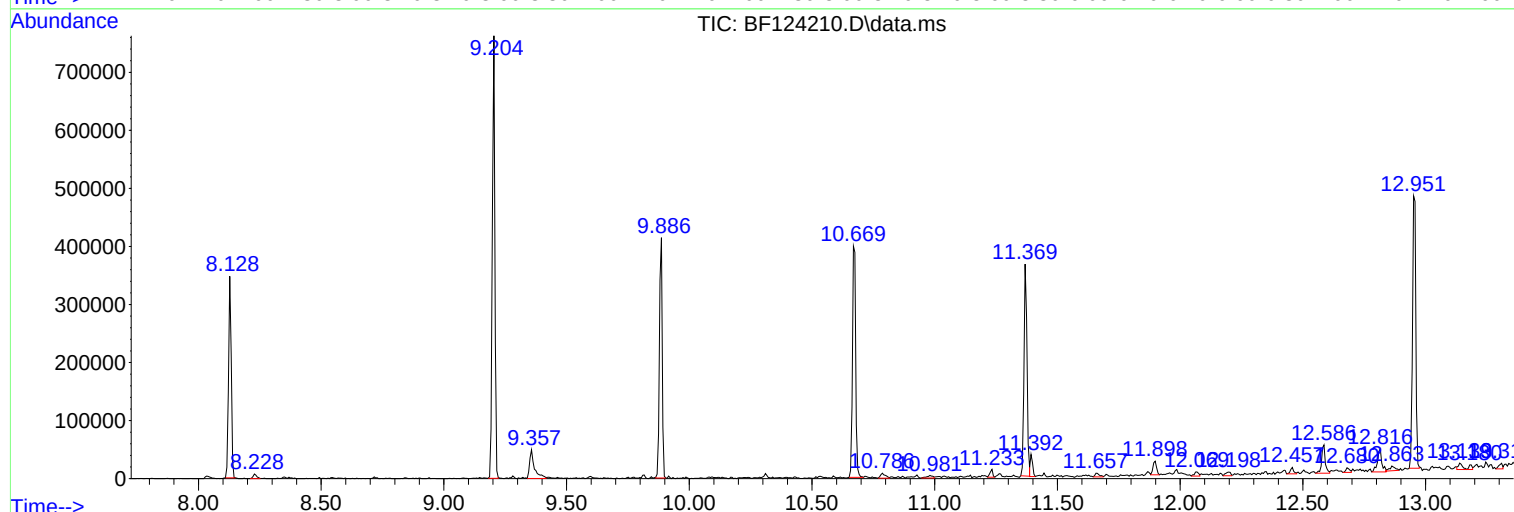
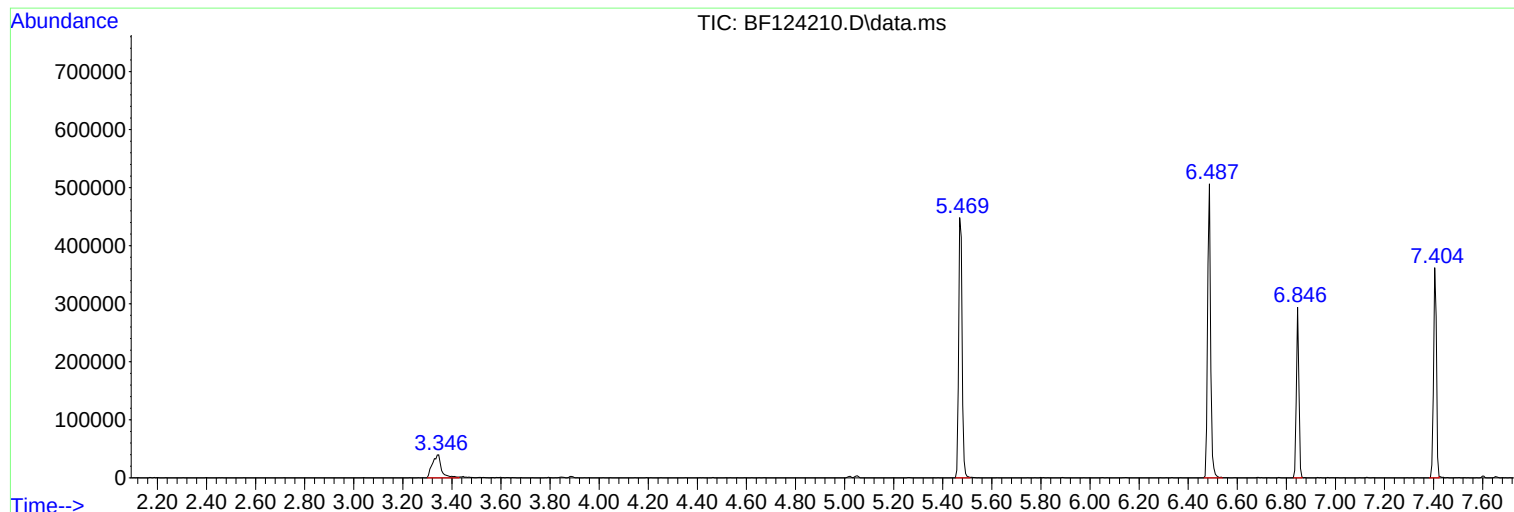
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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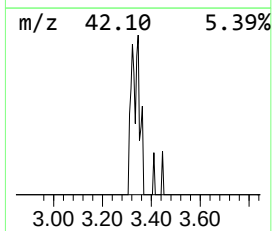
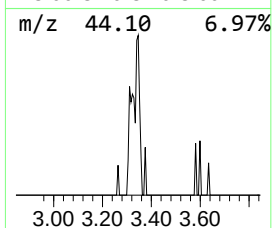
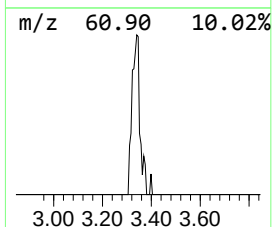
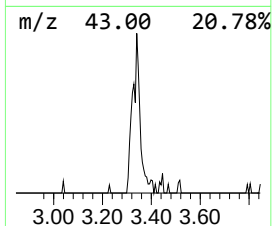
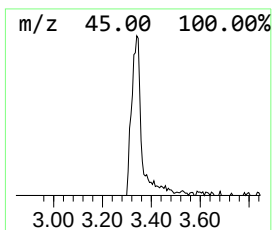
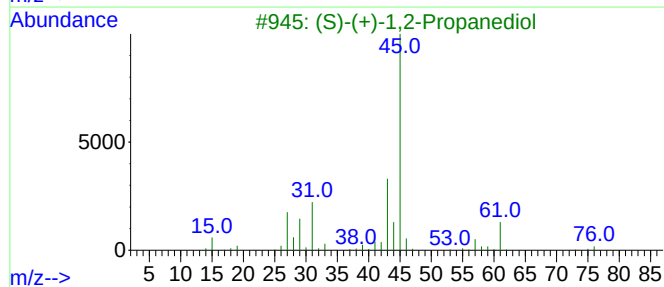
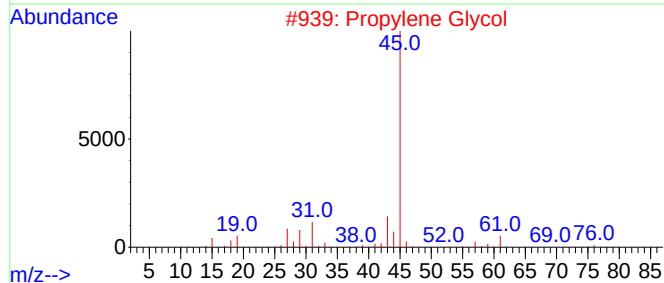
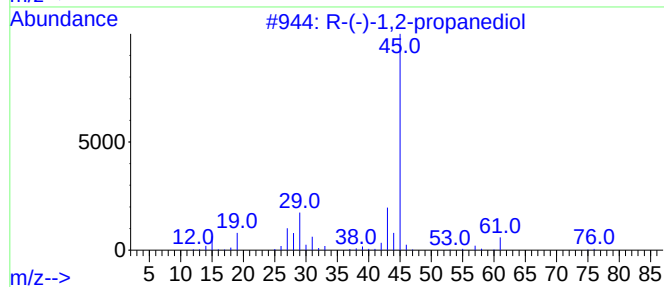
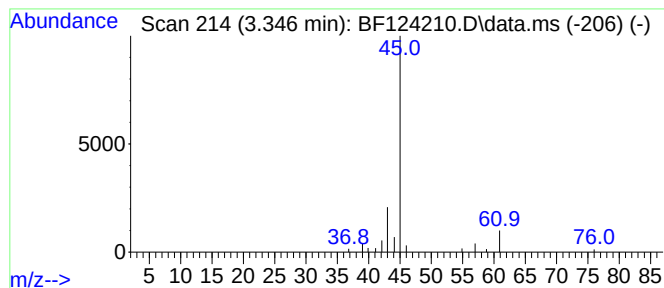
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 R-(-)-1,2-propanediol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.346	9.60 ng	102361	1,4-Dichlorobenzene-d4	6.846

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	86
2	Propylene Glycol			76	C3H8O2	000057-55-6	83
3	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	38
4	2-Pentanol, 3-methyl-			102	C6H14O	000565-60-6	9
5	Propane, 2-ethoxy-			88	C5H12O	000625-54-7	9



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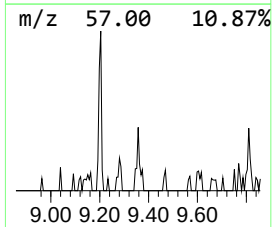
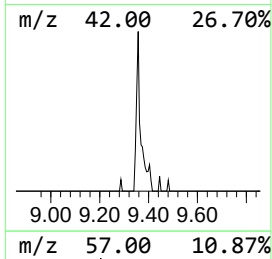
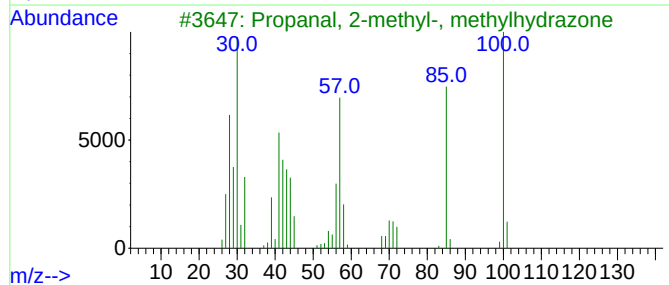
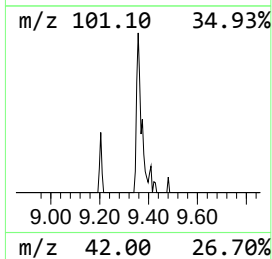
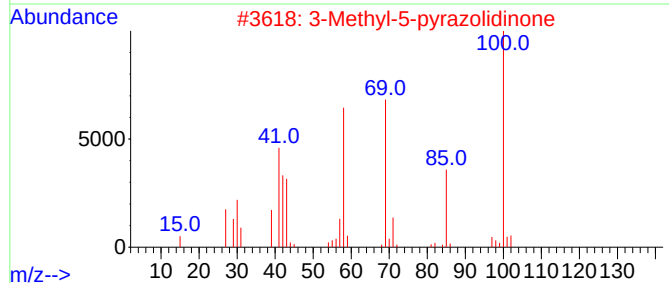
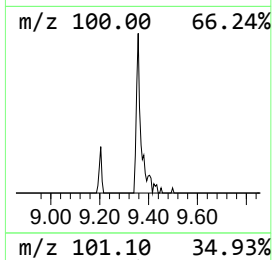
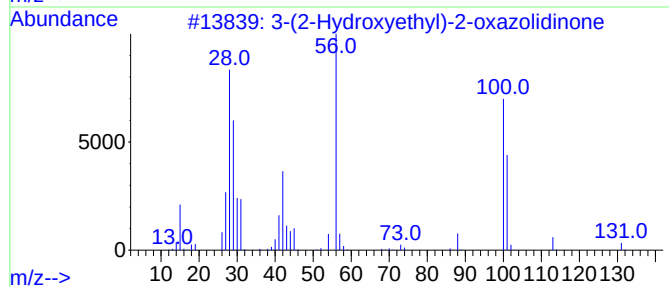
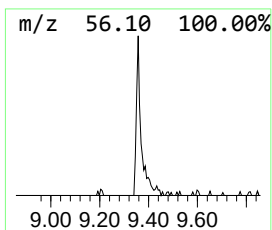
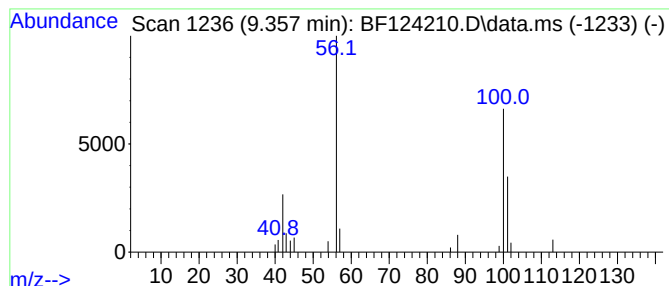
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-(2-Hydroxyethyl)-2-oxazol... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.357	4.14 ng	67779	Acenaphthene-d10	9.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-(2-Hydroxyethyl)-2-oxazolidinone	131	C5H9NO3	003356-88-5	83
2			3-Methyl-5-pyrazolidinone	100	C4H8N2O	010234-76-1	16
3			Propanal, 2-methyl-, methylhydra...	100	C5H12N2	016713-37-4	9
4			Cycloheptylamine	113	C7H15N	005452-35-7	9
5			Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	9



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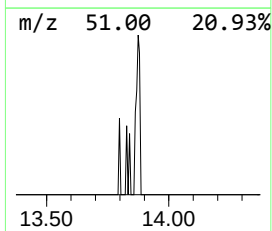
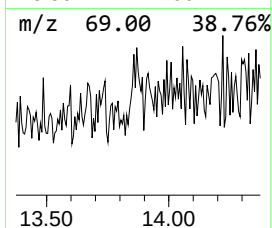
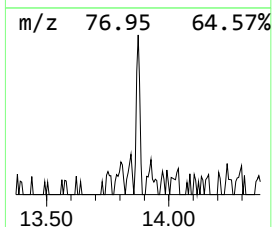
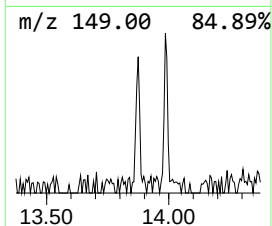
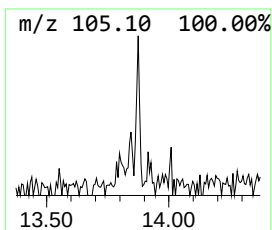
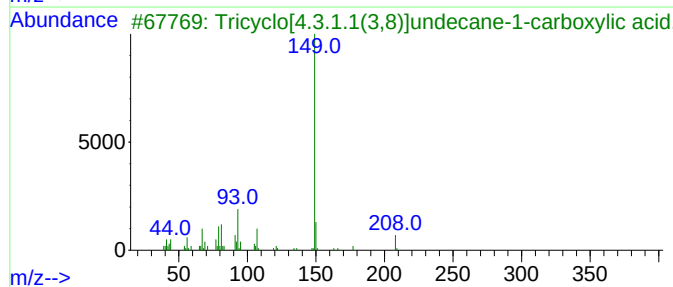
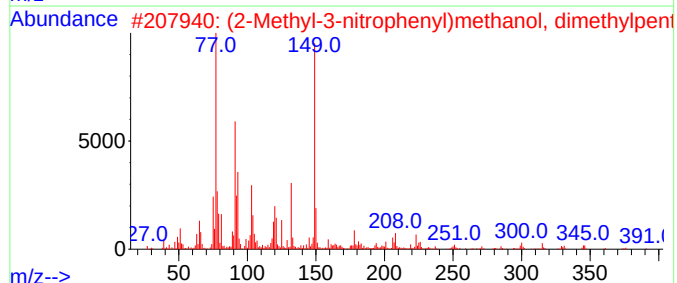
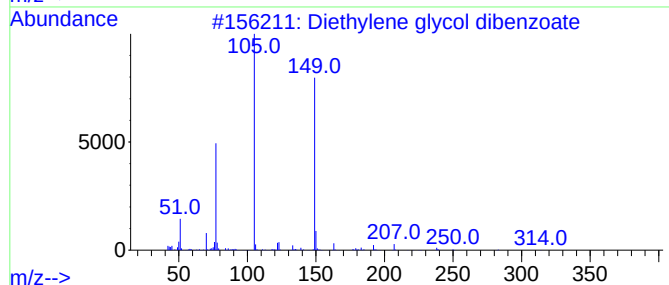
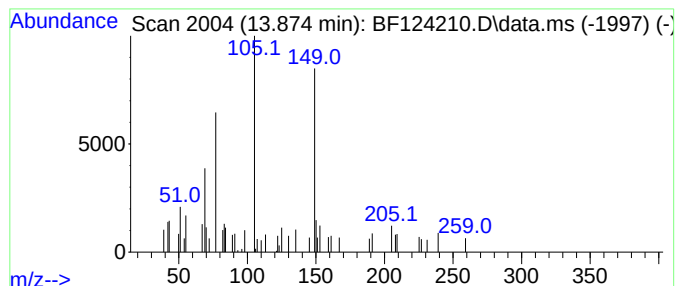
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Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	3.34 ng	54682	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	53
2			(2-Methyl-3-nitrophenyl)methanol...	391	C16H14F5NO3Si	1000367-95-1	42
3			Tricyclo[4.3.1.1(3,8)]undecane-1...	208	C13H20O2	031083-60-0	38
4			Oxazolidine, 3-phenyl-	149	C9H11NO	020503-92-8	38
5			Phthalic acid, butyl 3-methoxybe...	342	C20H22O5	1000377-97-7	37



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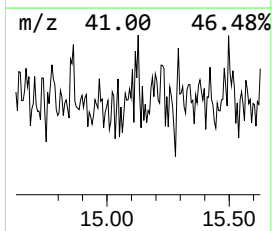
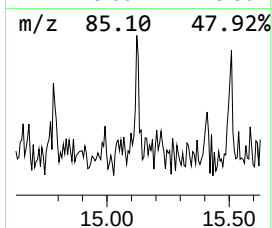
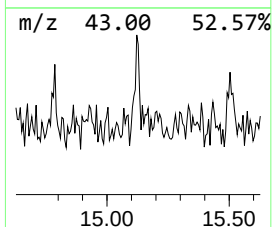
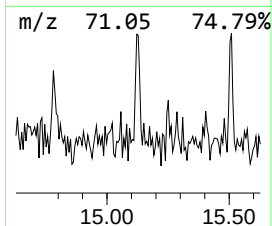
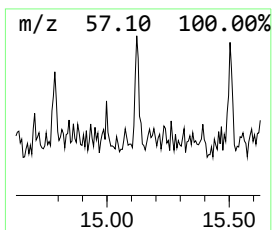
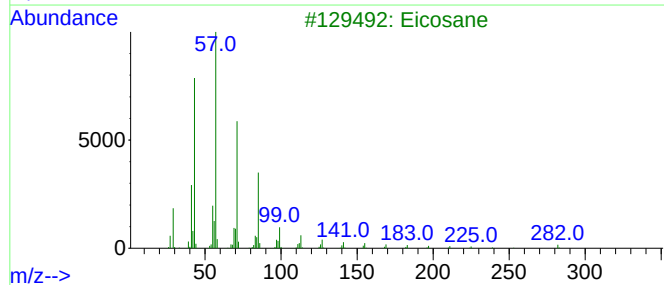
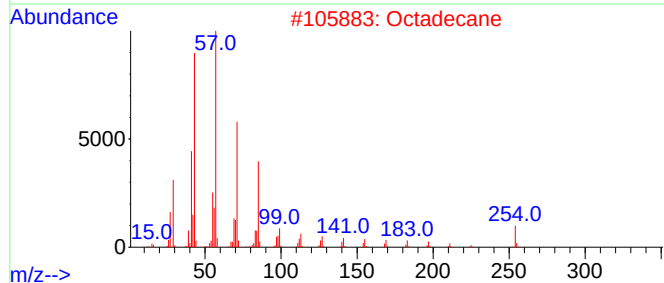
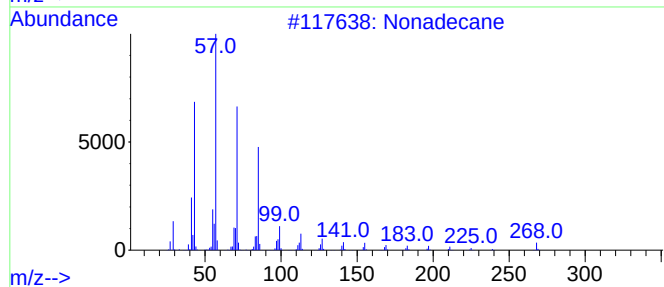
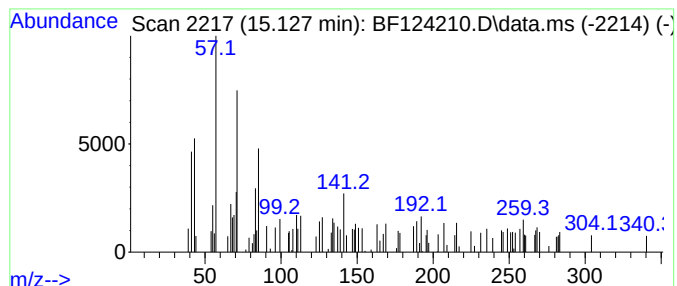
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Peak Number 6 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.127	2.67 ng	42412	Perylene-d12	15.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	58
2			Octadecane	254	C18H38	000593-45-3	58
3			Eicosane	282	C20H42	000112-95-8	53
4			Hexadecane, 1-bromo-	304	C16H33Br	000112-82-3	53
5			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	47



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17

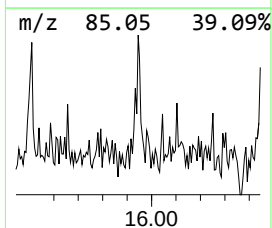
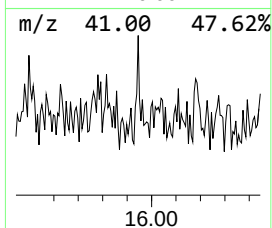
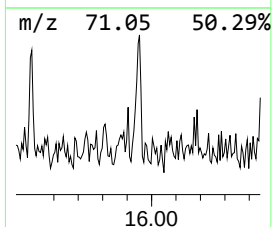
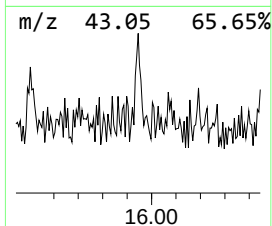
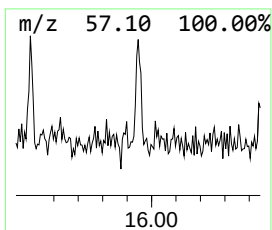
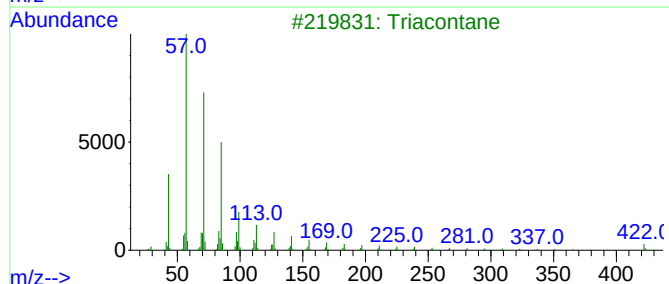
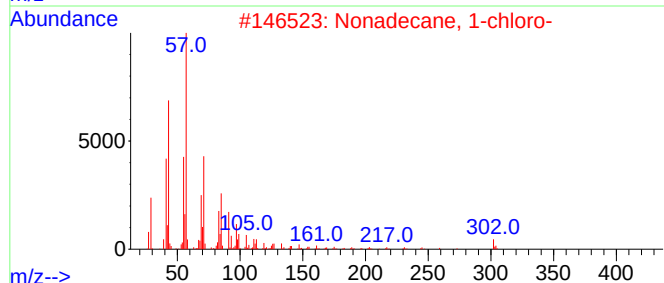
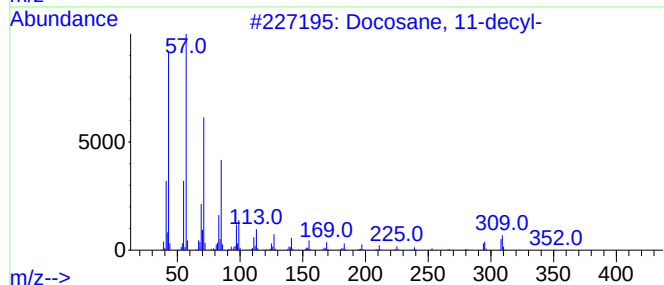
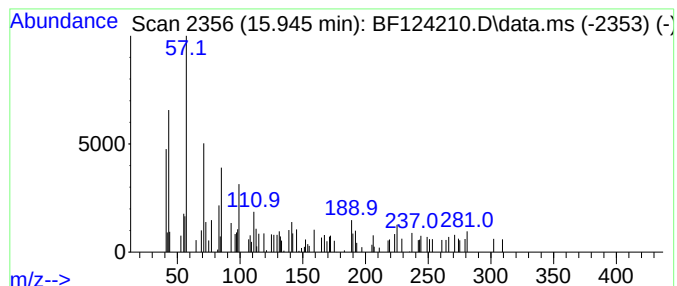
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.945 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	2.70 ng	42940	Perylene-d12	15.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane, 11-decyl-	451	C32H66	055401-55-3	49
2			Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	49
3			Triacontane	422	C30H62	000638-68-6	47
4			Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	47
5			Heneicosane	296	C21H44	000629-94-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124210.D
Acq On : 9 Jun 2021 15:49
Operator : JU/CG
Sample : M2598-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
17

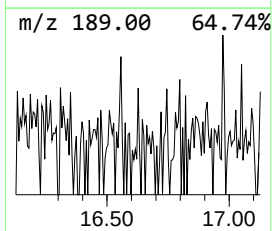
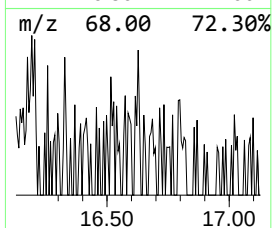
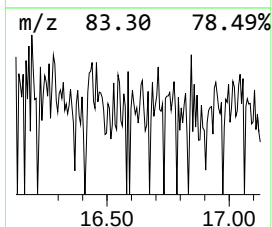
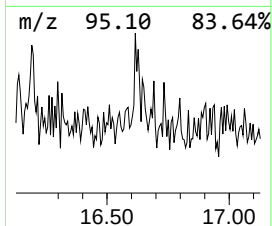
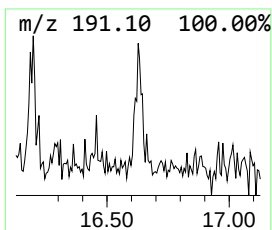
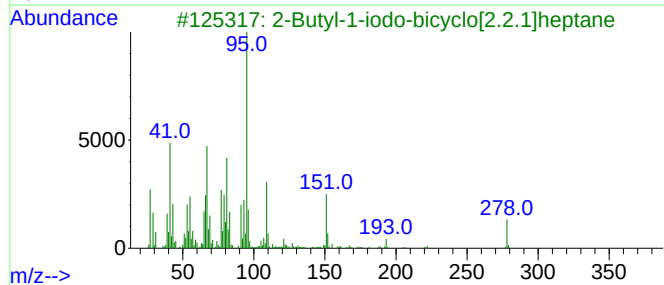
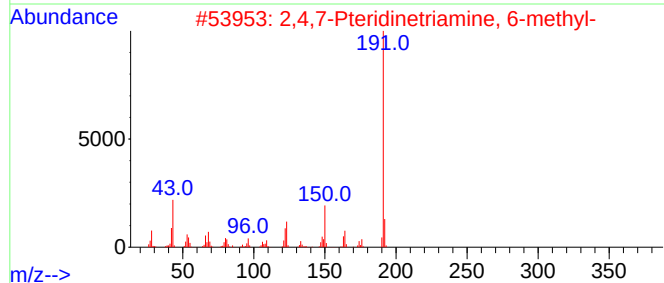
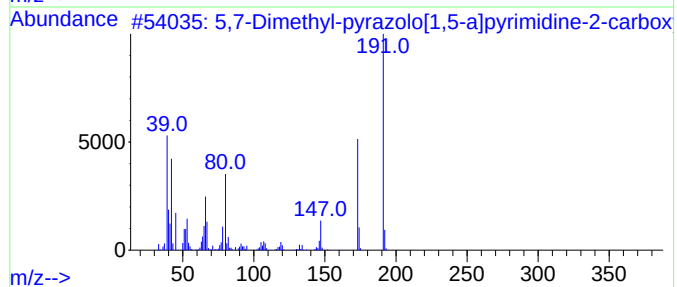
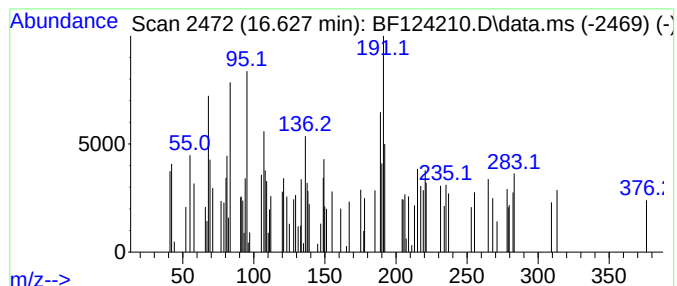
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.627 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.627	2.09 ng	33224	Perylene-d12	15.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5,7-Dimethyl-pyrazolo[1,5-a]pyri...	191	C9H9N3O2	1000303-40-5	25
2			2,4,7-Pteridinetriamine, 6-methyl-	191	C7H9N7	017539-50-3	22
3			2-Butyl-1-iodo-bicyclo[2.2.1]hep...	278	C11H19I	1000190-59-7	22
4			1,2,4-Triazolo[1,5-a]pyrimidine,...	212	C8H9FN4S	1000294-91-7	14
5			Cyclohexane, 1,2-dimethyl-3,5-bi...	192	C14H24	074806-56-7	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124210.D
Acq On : 9 Jun 2021 15:49
Operator : JU/CG
Sample : M2598-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
17

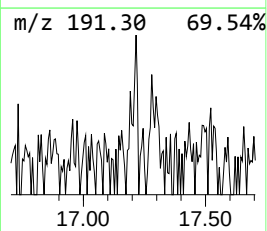
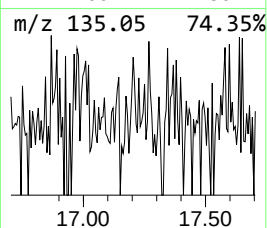
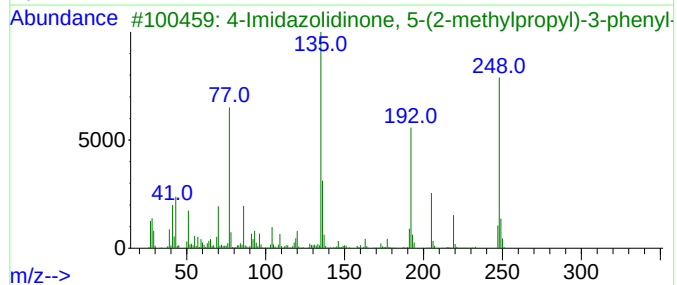
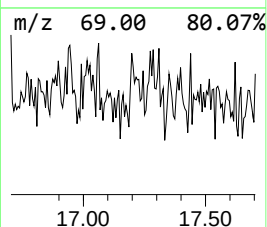
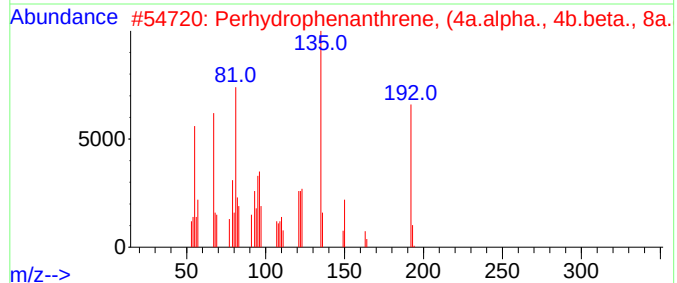
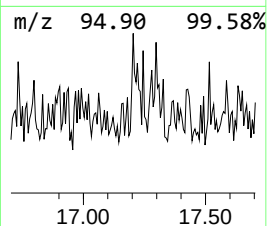
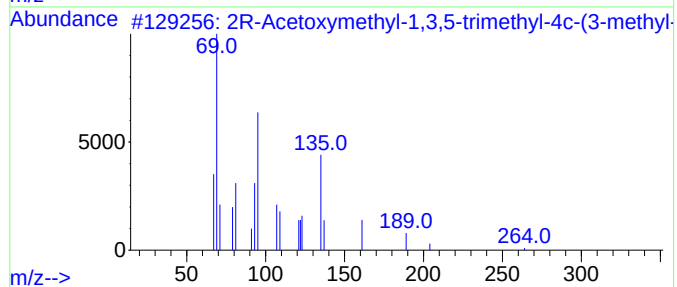
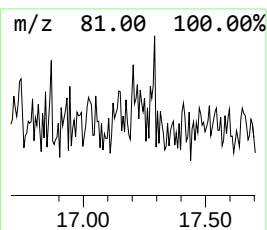
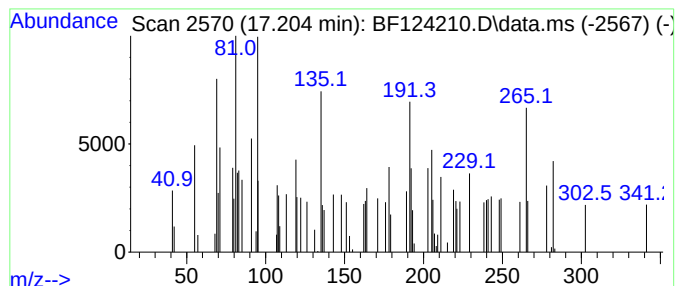
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.204 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.204	2.03 ng	32302	Perylene-d12	15.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2R-Acetoxyethyl-1,3,5-trimethyl...	282	C17H30O3	1000144-12-6	27
2			Perhydrophenanthrene, (4a.alpha....	192	C14H24	002108-89-6	22
3			4-Imidazolidinone, 5-(2-methylpr...	248	C13H16N2O5	004399-40-0	14
4			(3-Fluorophenyl)(furan-2-yl)meth...	192	C11H9FO2	1000305-63-1	12
5			2-Cyclopenten-1-one, 4-hydroxy-3...	178	C11H14O2	000487-67-2	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060921\
Data File : BF124210.D
Acq On : 9 Jun 2021 15:49
Operator : JU/CG
Sample : M2598-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
17

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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
R-(-)-1,2-propa...	3.346	9.6	ng	102361	1	6.846	213239	20.0
3-(2-Hydroxyeth...	9.357	4.1	ng	67779	3	9.886	327469	20.0
Diethylene glyc...	13.874	3.3	ng	54682	5	14.010	327420	20.0
Nonadecane	15.127	2.7	ng	42412	6	15.486	317637	20.0
unknown15.945	15.945	2.7	ng	42940	6	15.486	317637	20.0
unknown16.627	16.627	2.1	ng	33224	6	15.486	317637	20.0
unknown17.204	17.204	2.0	ng	32302	6	15.486	317637	20.0