

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091718\
 Data File : BG036768.D
 Acq On : 18 Sep 2018 1:25
 Operator : JU/SJ
 Sample : J4935-05
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PHASE-1-CONCRETE

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_G\METHODS\8270-BG082318.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	3.764	76	81	103	rBV	269498	423088	15.15%	2.224%
2	4.563	211	217	230	rBV	66785	107475	3.85%	0.565%
3	4.980	283	288	295	rVB2	17914	30554	1.09%	0.161%
4	5.156	312	318	328	rBV	146857	217345	7.78%	1.142%
5	5.620	389	397	409	rBV	644324	1035482	37.07%	5.442%
6	7.207	658	667	677	rBV	778223	1327276	47.52%	6.976%
7	7.583	724	731	743	rBV	661915	1131973	40.52%	5.949%
8	8.053	803	811	817	rBV	211778	362180	12.97%	1.904%
9	8.376	858	866	874	rVB	559847	976031	34.94%	5.130%
10	9.210	1000	1008	1016	rBV	472328	833444	29.84%	4.380%
11	10.144	1159	1167	1180	rBV	354940	604615	21.64%	3.178%
12	10.855	1280	1288	1296	rVB	292289	527111	18.87%	2.770%
13	13.035	1651	1659	1664	rBV	17290	29093	1.04%	0.153%
14	13.300	1695	1704	1712	rBV	1272561	2083605	74.59%	10.951%
15	14.122	1839	1844	1851	rVB	73553	102160	3.66%	0.537%
16	14.674	1929	1938	1948	rBV2	455733	742259	26.57%	3.901%
17	16.161	2183	2191	2205	rBV	658494	1019668	36.50%	5.359%
18	17.418	2398	2405	2411	rBV2	617644	918767	32.89%	4.829%
19	17.777	2461	2466	2473	rBV	12252	28770	1.03%	0.151%
20	20.027	2843	2849	2856	rBV	1986217	2793359	100.00%	14.681%
21	20.820	2980	2984	2988	rBV4	25410	32805	1.17%	0.172%
22	21.325	3066	3070	3076	rBV3	56740	97003	3.47%	0.510%
23	21.566	3107	3111	3119	rVB	107468	152568	5.46%	0.802%
24	21.684	3124	3131	3139	rVV2	598648	995677	35.64%	5.233%
25	21.878	3160	3164	3171	rVB2	31684	41796	1.50%	0.220%
26	22.483	3263	3267	3272	rBV2	34080	48455	1.73%	0.255%
27	23.176	3380	3385	3391	rBV3	38043	99231	3.55%	0.522%
28	23.370	3413	3418	3423	rBV3	76604	157684	5.64%	0.829%
29	24.293	3569	3575	3586	rVB4	218554	789788	28.27%	4.151%
30	24.892	3672	3677	3690	rVB2	416766	1238241	44.33%	6.508%
31	26.043	3869	3873	3881	rVB5	30980	79076	2.83%	0.416%

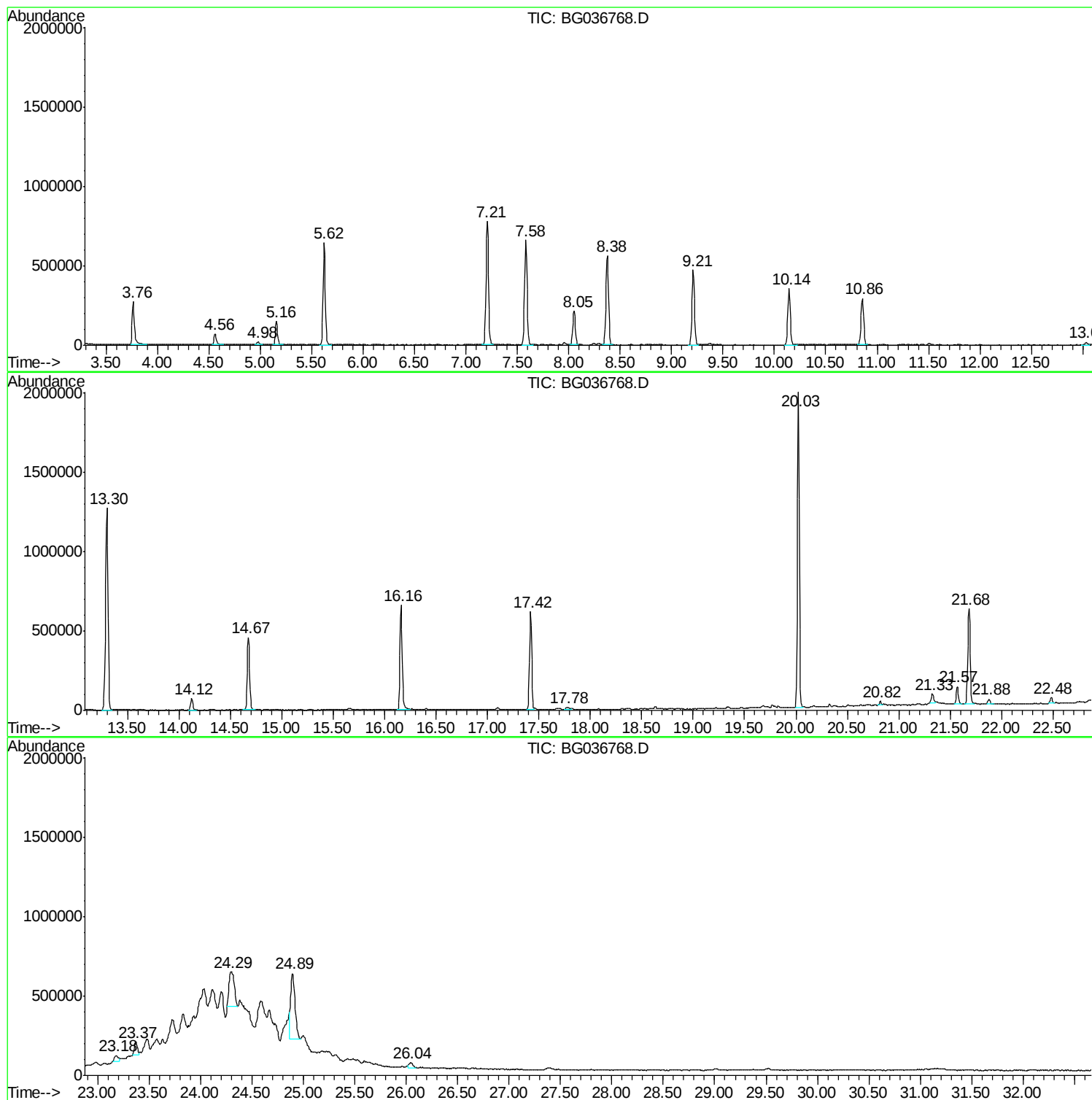
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PHASE-1-CONCRETE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.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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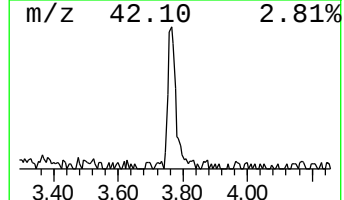
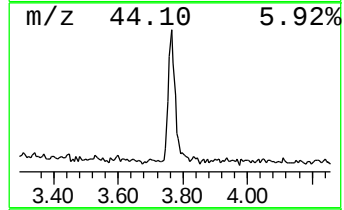
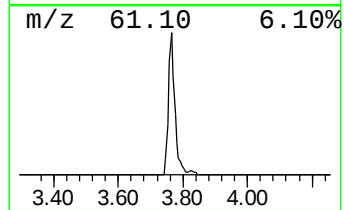
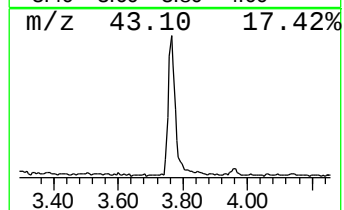
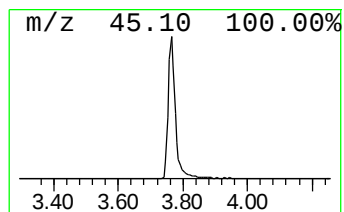
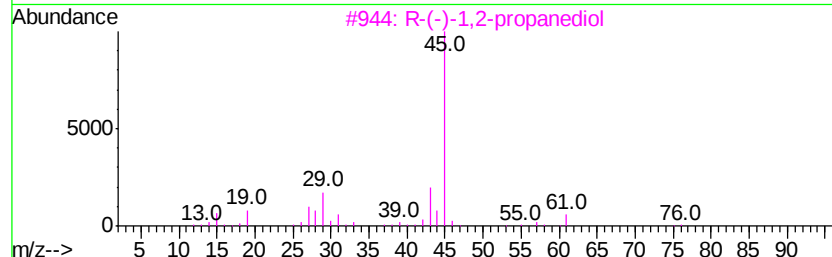
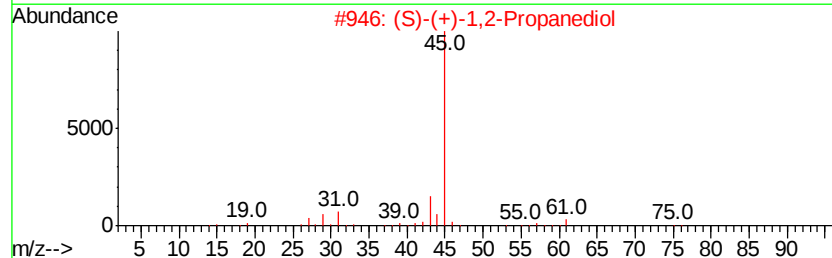
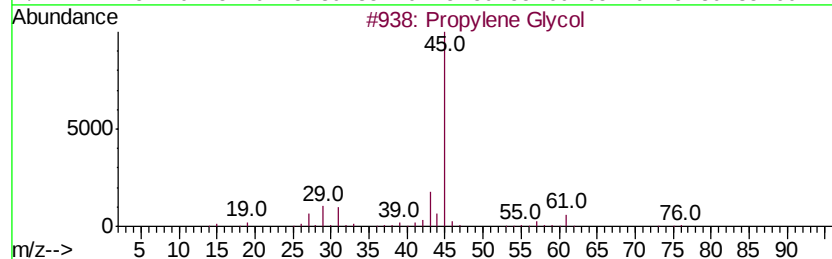
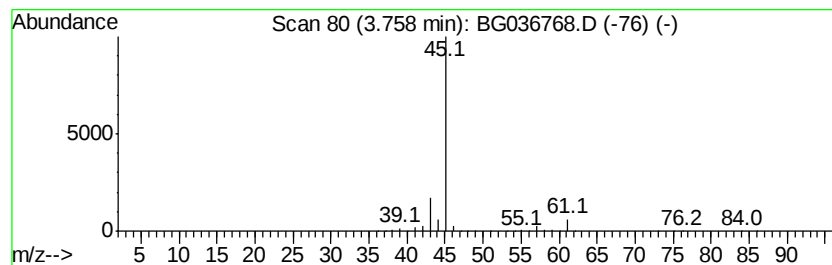
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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Peak Number 1 Propylene Glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.76	23.36 ng	423088	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propylene Glycol	76	C3H8O2	000057-55-6	78
2		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
4		2-Butanol, (R)-	74	C4H10O	014898-79-4	9
5		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9



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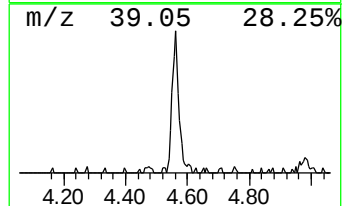
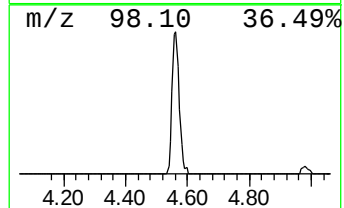
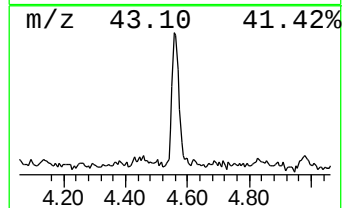
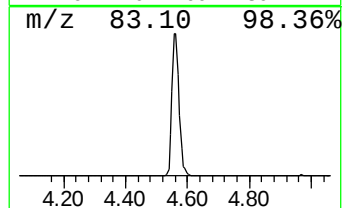
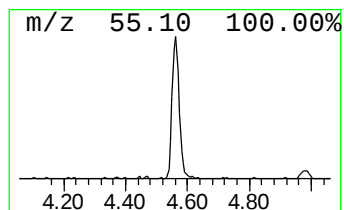
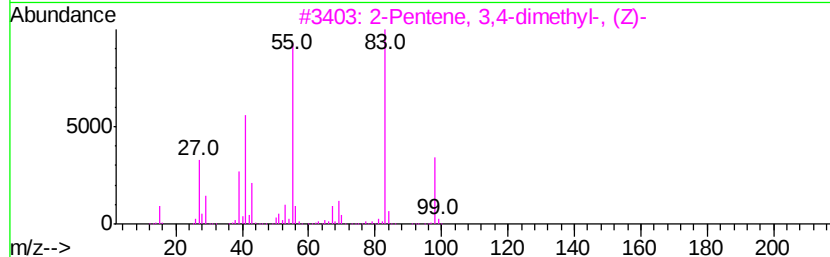
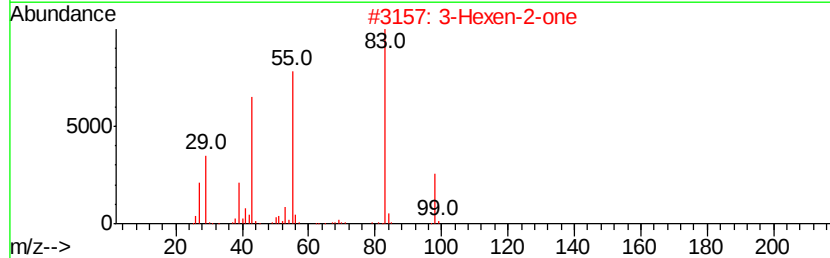
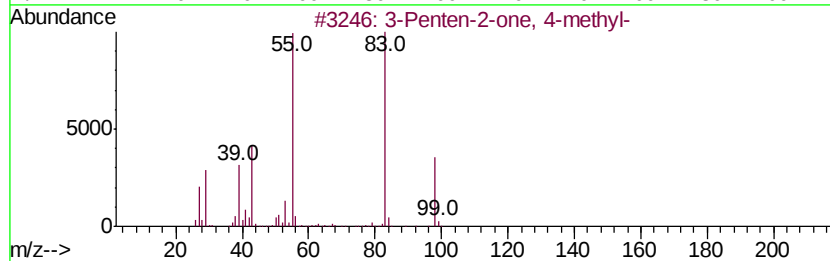
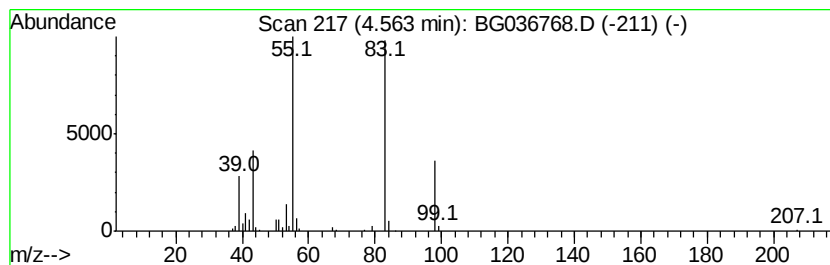
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	5.93 ng	107475	1,4-Dichlorobenzene-d4	8.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	87
3			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
5			2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	72



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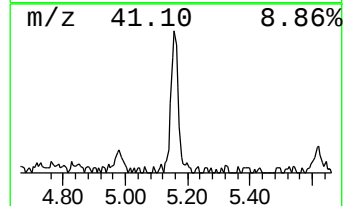
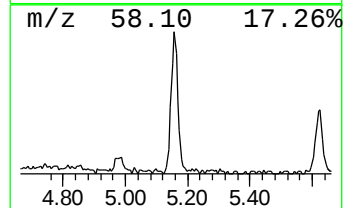
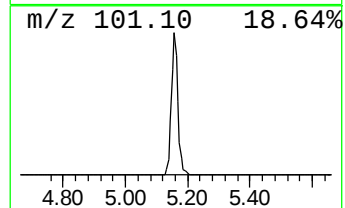
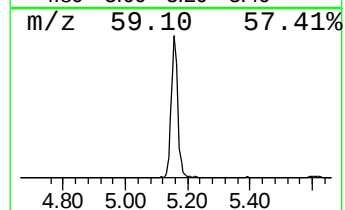
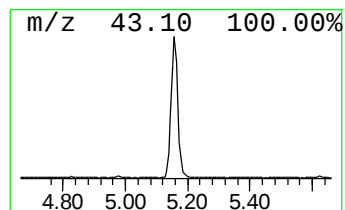
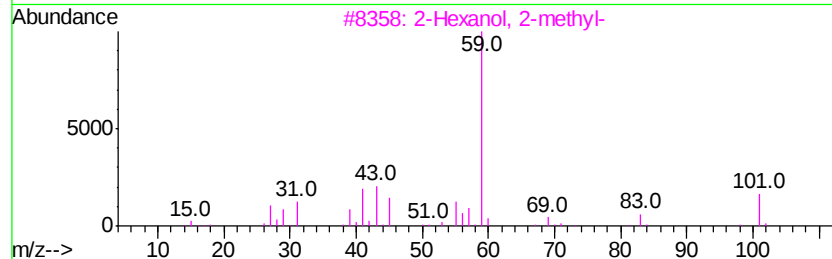
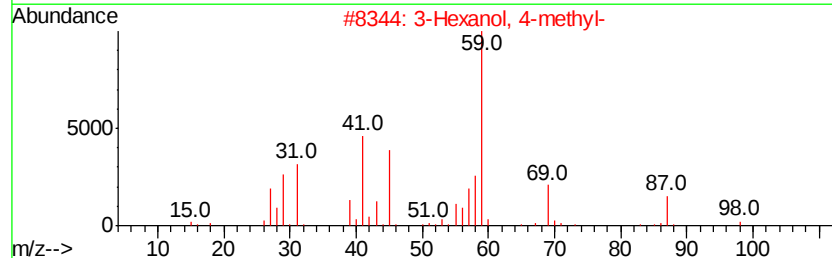
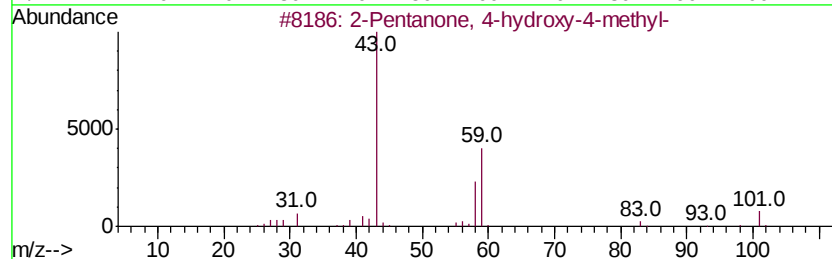
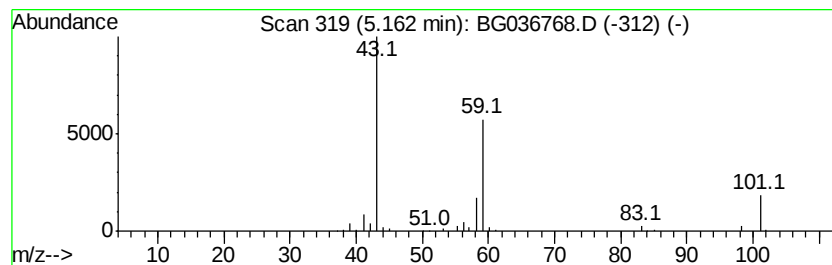
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	12.00 ng	217345	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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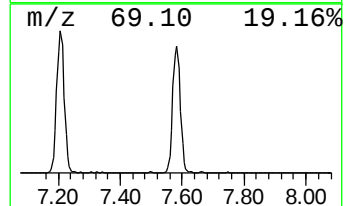
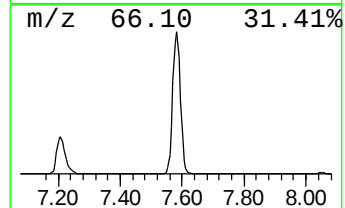
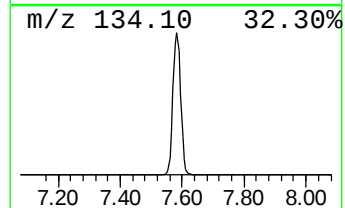
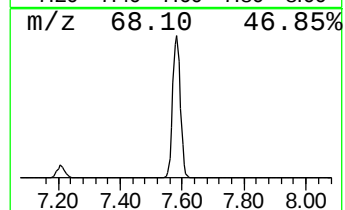
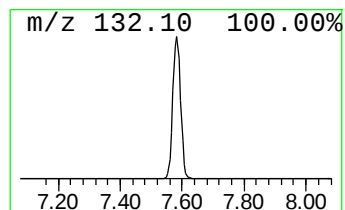
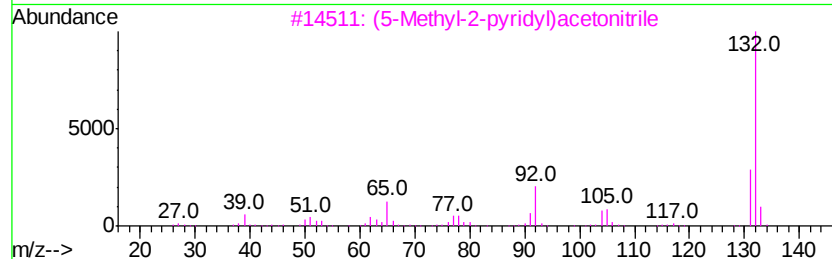
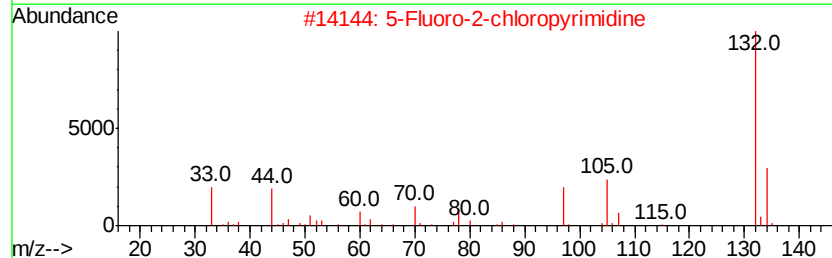
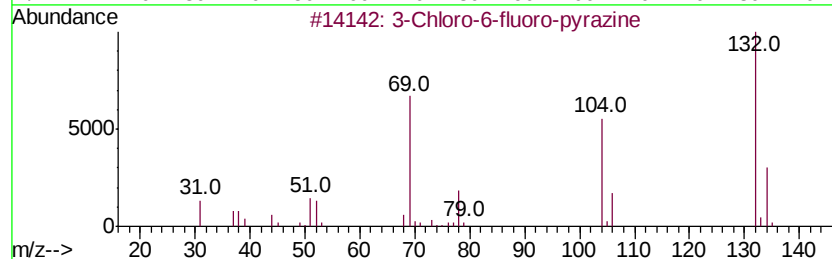
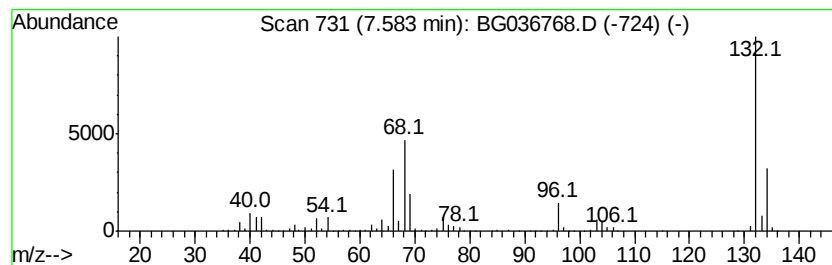
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Peak Number 4 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	62.51 ng	1131970	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		5-Aminoindole	132	C8H8N2	005192-03-0	10



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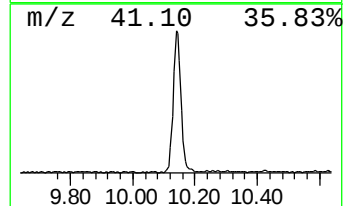
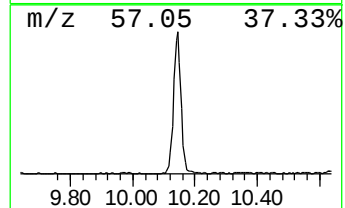
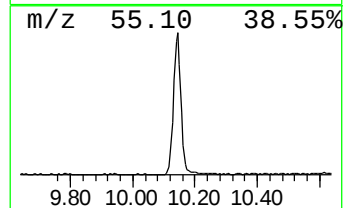
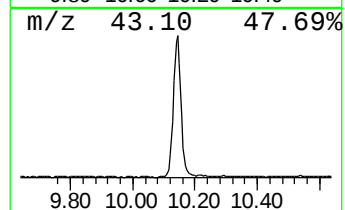
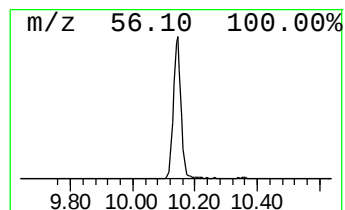
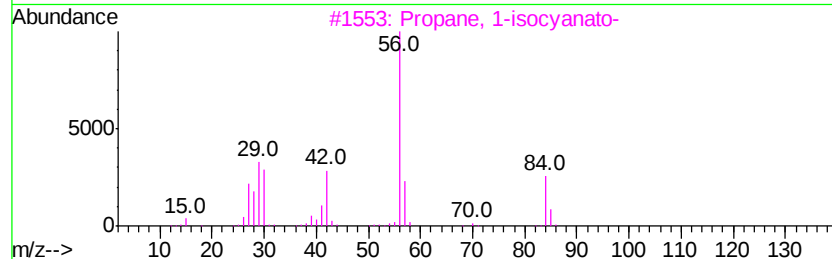
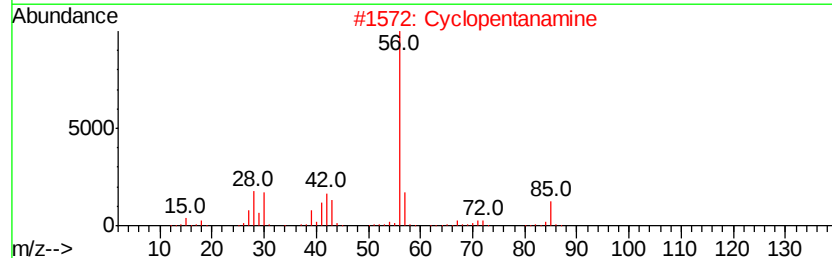
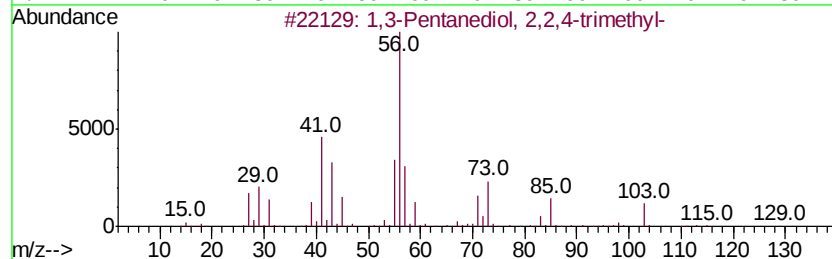
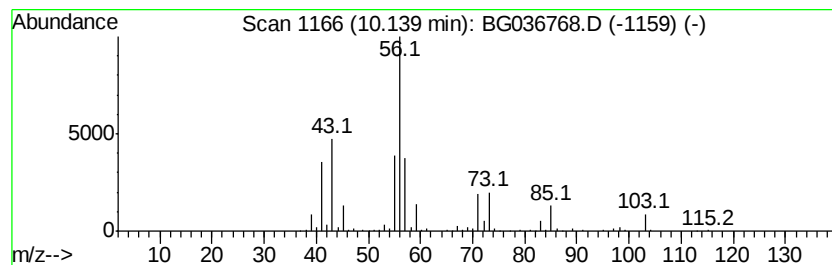
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Peak Number 6 1,3-Pentanediol, 2,2,4-trim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.14	22.94 ng	604615	Naphthalene-d8	10.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	80
2		Cyclopentanamine	85	C5H11N	001003-03-8	38
3		Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	37
4		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	37
5		3,3-Diethyldiaziridine	100	C5H12N2	052175-94-7	33



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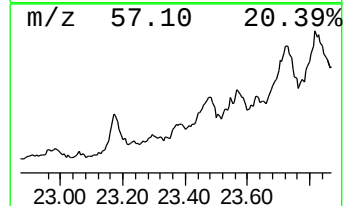
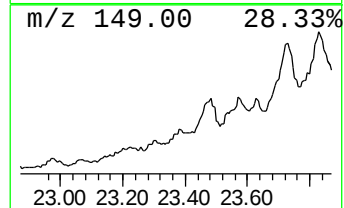
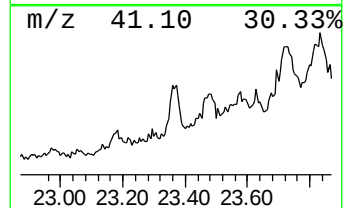
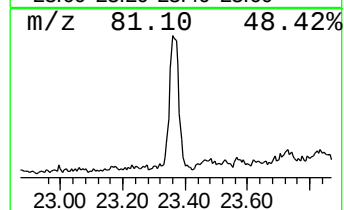
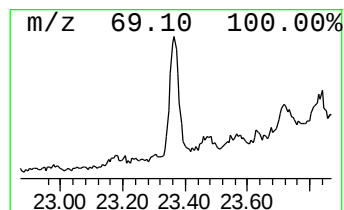
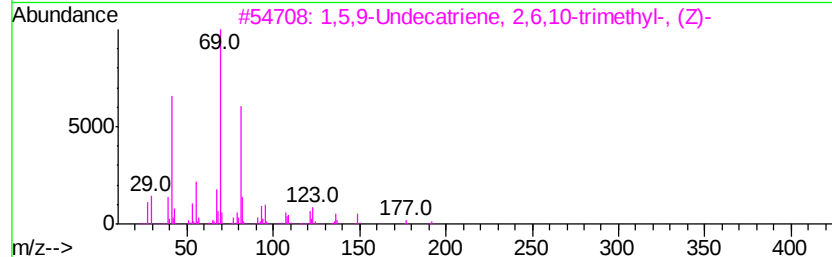
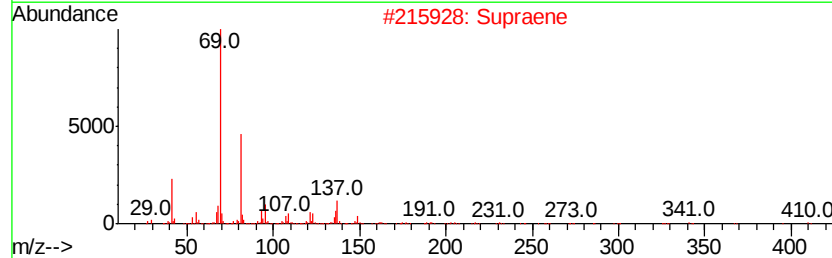
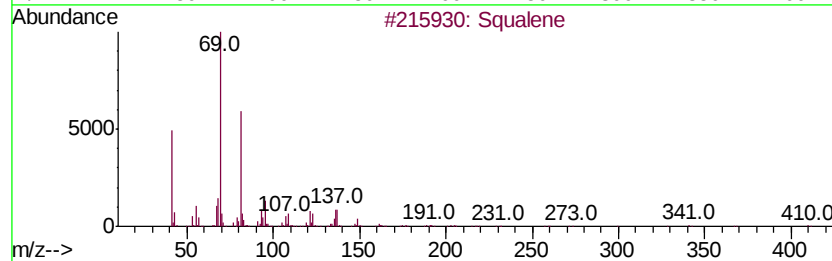
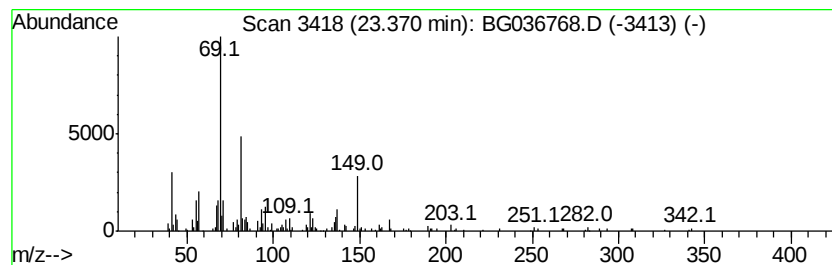
Instrument :
BNA_G
ClientSampleId :
PHASE-1-CONCRETE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.37	2.55 ng	157684	Perylene-d12	24.89
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	000111-02-4	76
2	Supraene	410 C30H50	007683-64-9	74
3	1,5,9-Undecatriene, 2,6,10-trime...	192 C14H24	062951-96-6	58
4	trans-Farnesol	222 C15H26O	000106-28-5	58
5	Trifluoroacetyl-lavandulol	250 C12H17F3O2	028673-24-7	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091718\
Data File : BG036768.D
Acq On : 18 Sep 2018 1:25
Operator : JU/SJ
Sample : J4935-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

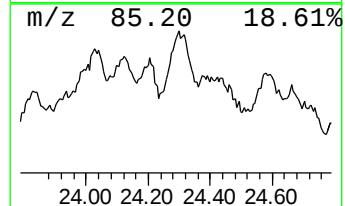
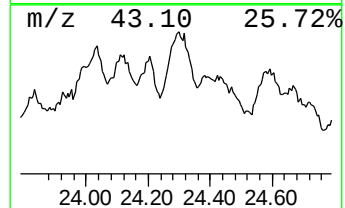
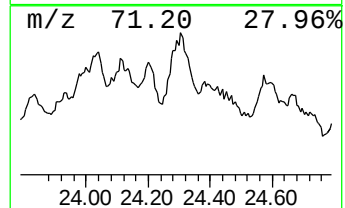
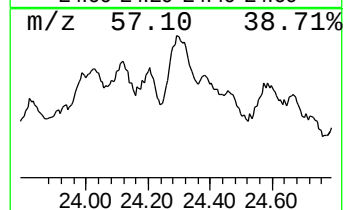
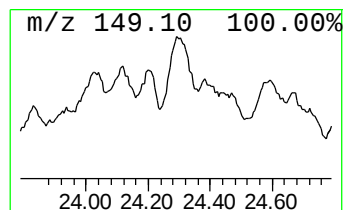
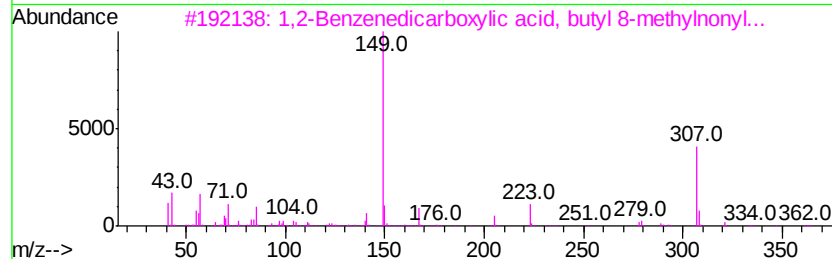
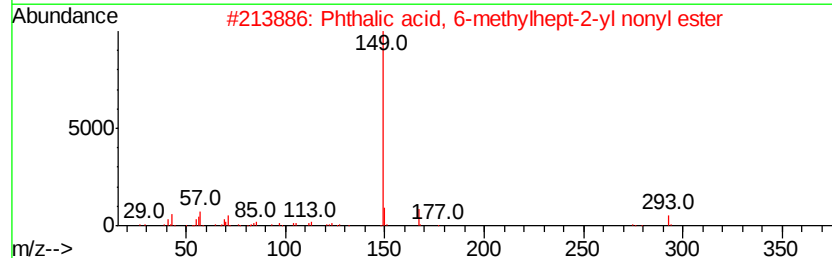
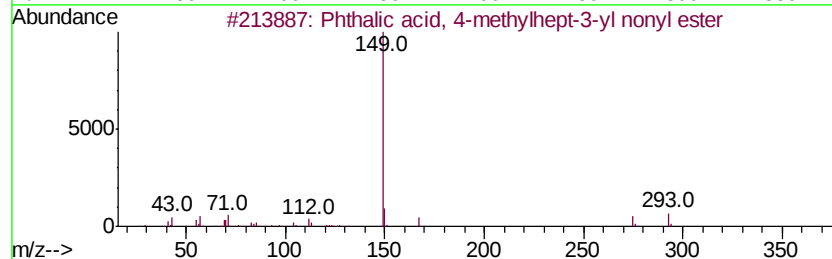
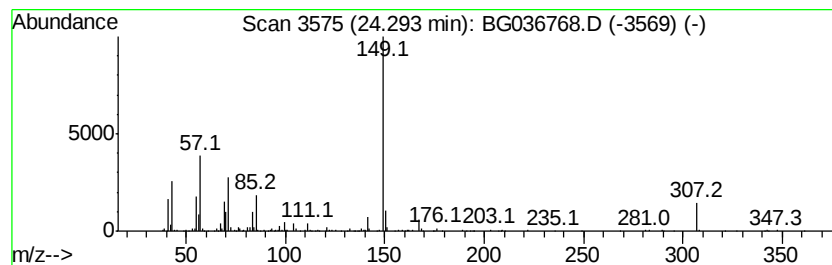
Instrument :
BNA_G
ClientSampleId :
PHASE-1-CONCRETE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phthalic acid, 4-methylhept... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
24.29	12.76 ng	789788	Perylene-d12	24.89		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, 4-methylhept-3-yl...	404	C25H40O4	1000377-94-4	64	
2	Phthalic acid, 6-methylhept-2-yl...	404	C25H40O4	1000377-96-3	64	
3	1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-18-9	64	
4	Didecyl phthalate	446	C28H46O4	000084-77-5	59	
5	1,2-Benzenedicarboxylic acid, bi...	334	C20H30O4	000146-50-9	53	



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG091718\
Data File : BG036768.D
Acq On : 18 Sep 2018 1:25
Operator : JU/SJ
Sample : J4935-05
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PHASE-1-CONCRETE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.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
Propylene Glycol	3.76	23.4	ng	423088	1	8.05	362180	20.0
3-Penten-2-one, 4...	4.56	5.9	ng	107475	1	8.05	362180	20.0
2-Pentanone, 4-hy...	5.16	12.0	ng	217345	1	8.05	362180	20.0
unknown7.58	7.58	62.5	ng	1131970	1	8.05	362180	20.0
1,3-Pentanediol, ...	10.14	22.9	ng	604615	2	10.86	527111	20.0
Squalene	23.37	2.5	ng	157684	6	24.89	1238240	20.0
Phthalic acid, 4-...	24.29	12.8	ng	789788	6	24.89	1238240	20.0