

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080817\
 Data File : BF097497.D
 Acq On : 9 Aug 2017 4:38
 Operator : SJ/JU
 Sample : I4604-03
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1-080217

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:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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	4.534	464	467	484	rBV	42158	81523	3.59%	0.486%
2	5.004	544	547	565	rBV	890330	1350568	59.52%	8.052%
3	6.081	727	730	743	rVB	578405	770936	33.98%	4.596%
4	6.181	743	747	757	rVB	2090494	2079910	91.67%	12.400%
5	6.404	782	785	796	rBV	569887	536208	23.63%	3.197%
6	6.563	808	812	827	rBV	2034062	2036406	89.75%	12.140%
7	6.981	879	883	901	rBV	1674861	1674986	73.82%	9.986%
8	7.687	1000	1003	1016	rBV	754925	733766	32.34%	4.374%
9	8.769	1183	1187	1190	rBV	2522903	2269013	100.00%	13.527%
10	9.169	1252	1255	1259	rBV	71826	66369	2.93%	0.396%
11	9.434	1296	1300	1311	rBV	688503	631346	27.82%	3.764%
12	10.222	1430	1434	1446	rBV	1158907	1140313	50.26%	6.798%
13	10.357	1454	1457	1464	rVB2	20401	26163	1.15%	0.156%
14	10.904	1547	1550	1559	rBV	501137	472417	20.82%	2.816%
15	11.151	1589	1592	1597	rBV	24986	34405	1.52%	0.205%
16	11.469	1643	1646	1652	rBV2	31997	49512	2.18%	0.295%
17	12.251	1775	1779	1782	rBV4	29872	32911	1.45%	0.196%
18	12.298	1782	1787	1790	rVV	45266	63869	2.81%	0.381%
19	12.492	1815	1820	1823	rBV	1703209	1638820	72.23%	9.770%
20	13.298	1954	1957	1960	rVB2	21628	24561	1.08%	0.146%
21	13.433	1977	1980	1984	rBV6	24838	36943	1.63%	0.220%
22	13.533	1993	1997	2001	rVB	496988	464270	20.46%	2.768%
23	13.880	2053	2056	2057	rBV3	20710	25871	1.14%	0.154%
24	14.874	2221	2225	2229	rBV	318760	355235	15.66%	2.118%
25	14.957	2237	2239	2243	rBV4	26207	43957	1.94%	0.262%
26	15.180	2275	2277	2281	rBV4	22051	39482	1.74%	0.235%
27	16.086	2425	2431	2433	rBV5	34845	61164	2.70%	0.365%
28	16.280	2461	2464	2467	rBV4	21149	33128	1.46%	0.197%

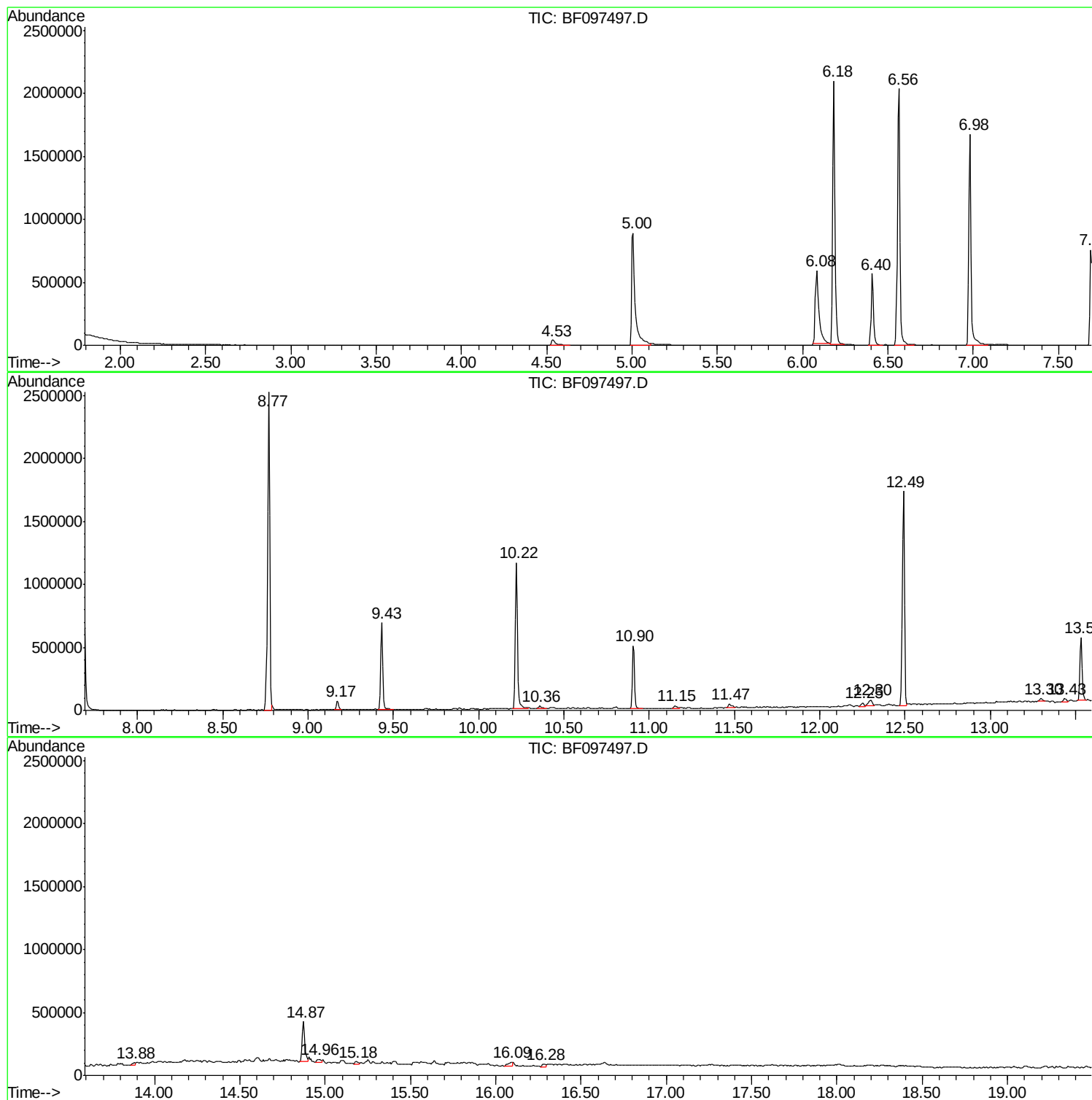
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Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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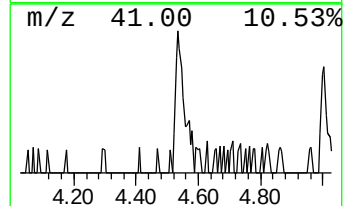
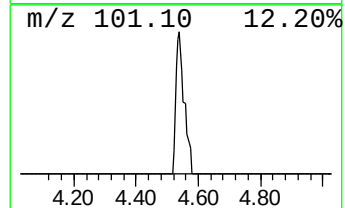
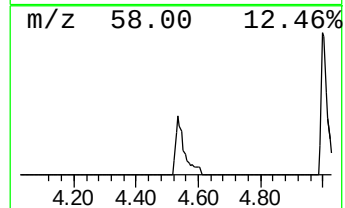
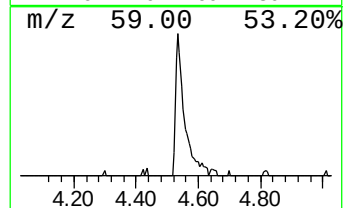
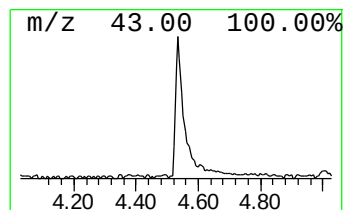
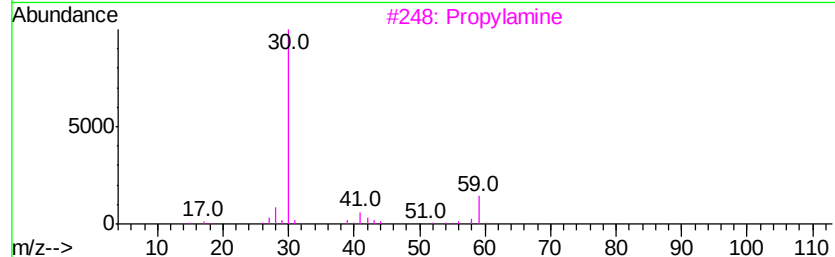
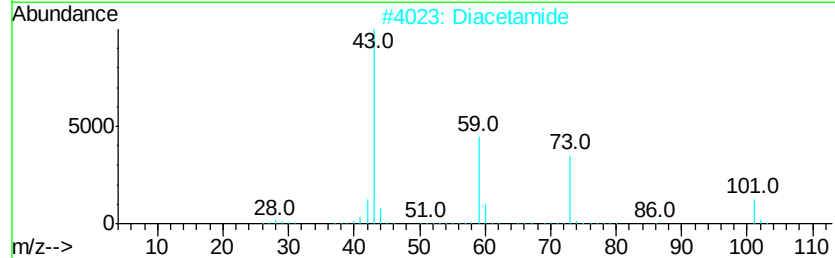
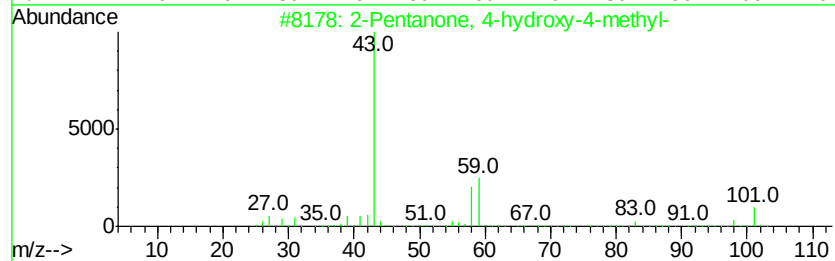
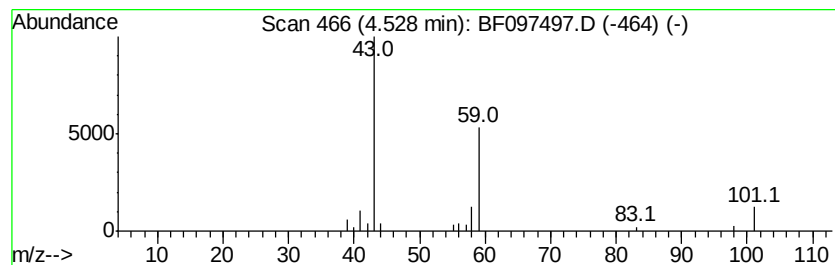
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	3.04 ng	81523	1,4-Dichlorobenzene-d4	6.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Diacetamide	101	C4H7NO2	000625-77-4	9
3		Propylamine	59	C3H9N	000107-10-8	9
4		2-Heptanone, 7,7-dichloro-	182	C7H12Cl2O	066241-43-8	9
5		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9



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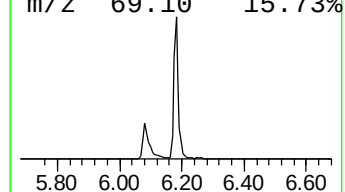
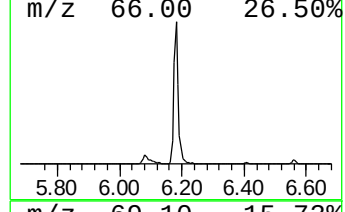
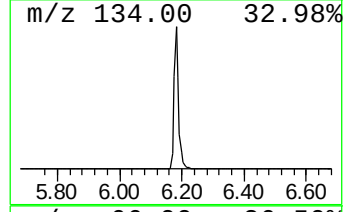
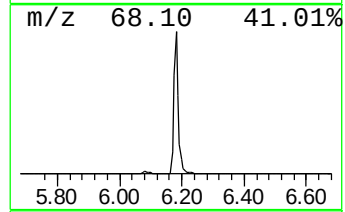
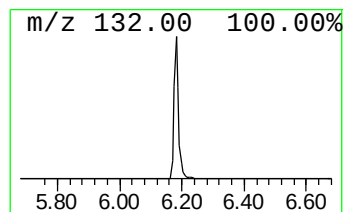
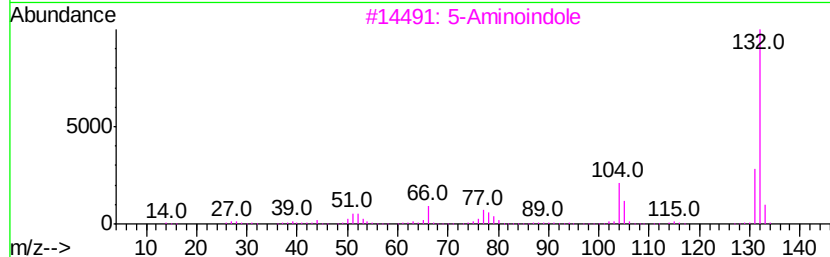
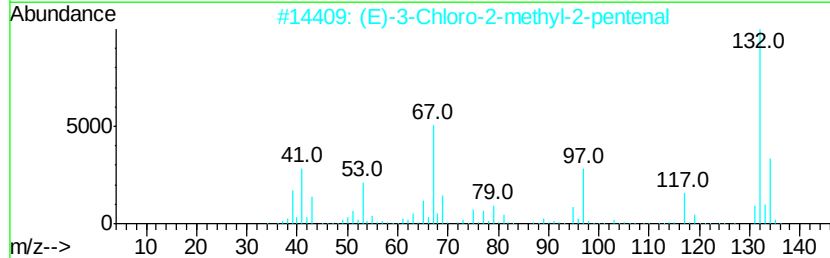
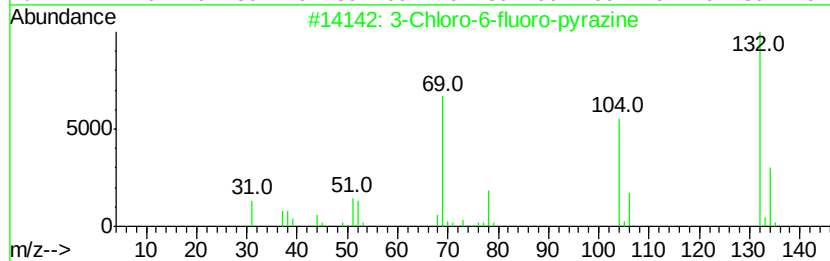
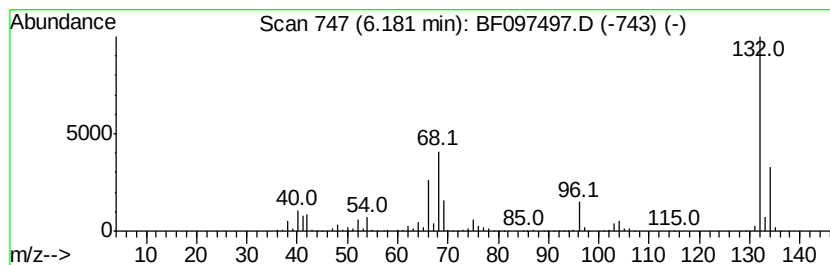
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Peak Number 2 unknown6.18 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.18	77.58 ng	2079910	1,4-Dichlorobenzene-d4	6.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3			5-Aminoindole	132	C8H8N2	005192-03-0	12
4			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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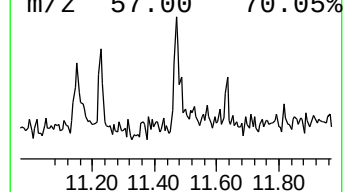
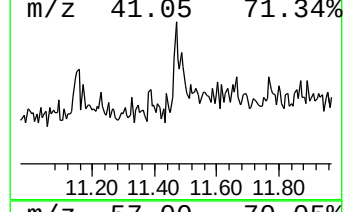
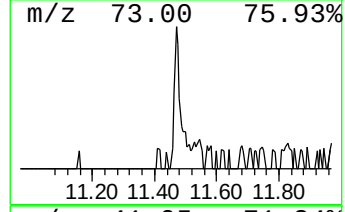
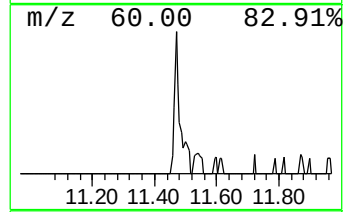
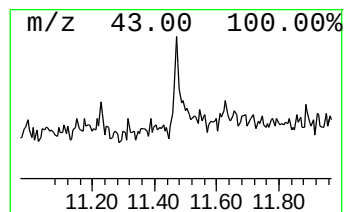
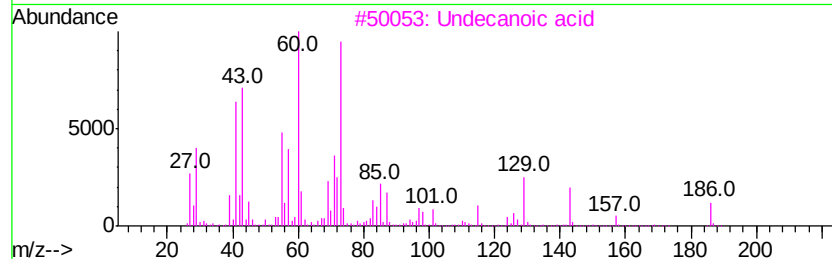
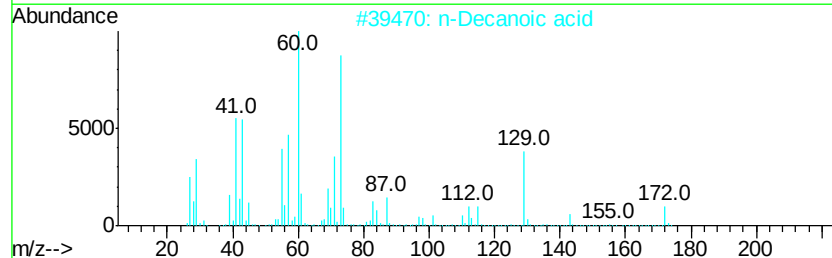
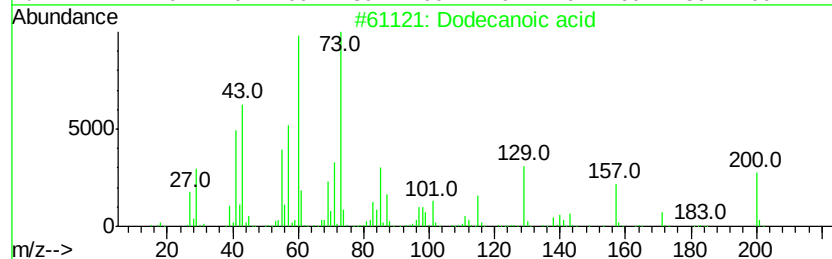
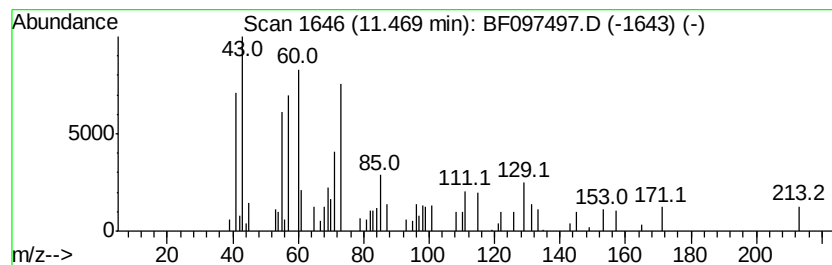
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Peak Number 4 Dodecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	2.10 ng	49512	Phenanthrene-d10	10.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid	200	C12H24O2	000143-07-7	53
2		n-Decanoic acid	172	C10H20O2	000334-48-5	50
3		Undecanoic acid	186	C11H22O2	000112-37-8	50
4		d-Glucohexodialdose	178	C6H10O6	1000149-19-1	38
5		Sedoheptulosan	192	C7H12O6	000469-90-9	27



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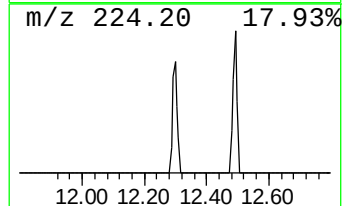
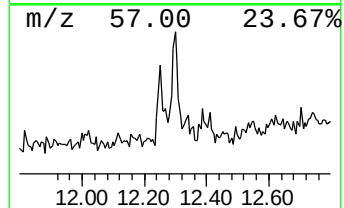
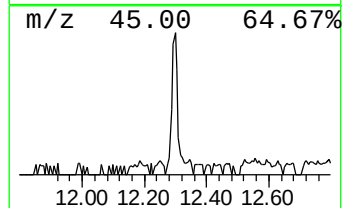
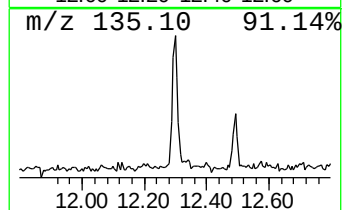
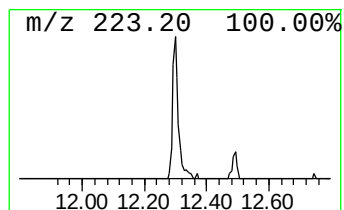
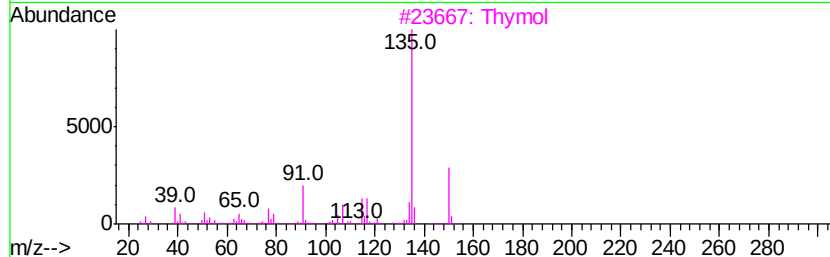
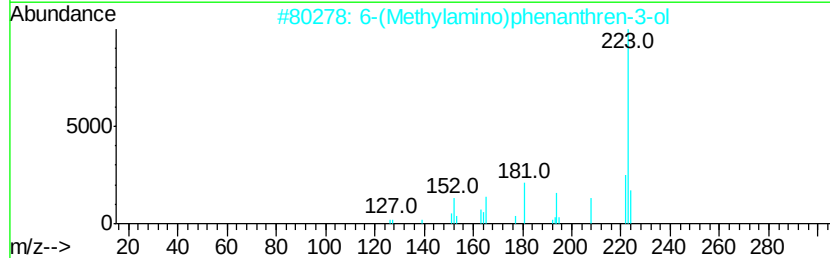
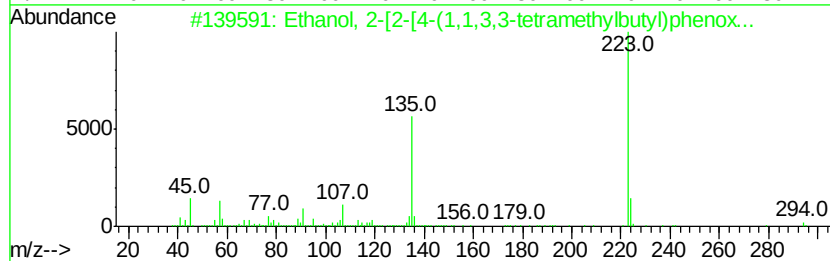
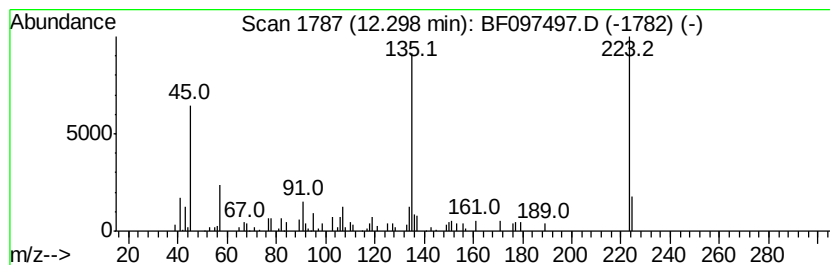
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Peak Number 5 unknown12.30 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	2.75 ng	63869	Chrysene-d12	13.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-[2-[4-(1,1,3,3-tetram...	294	C18H30O3	002315-61-9	47
2		6-(Methylamino)phenanthren-3-ol	223	C15H13NO	098033-23-9	35
3		Thymol	150	C10H14O	000089-83-8	27
4		2-Methyl-2-(4'-hydroxyphenyl)pen...	192	C12H16O2	070205-18-4	25
5		Pyrido[1,2-a]benzimidazol-4-carb...	223	C13H9N3O	060792-57-6	22



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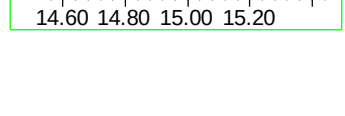
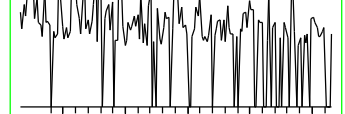
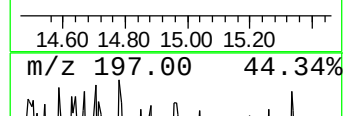
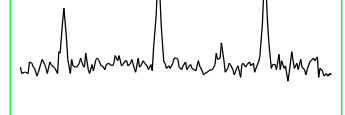
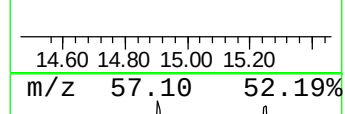
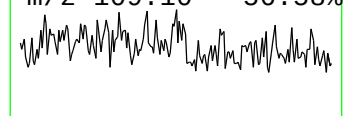
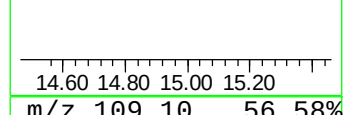
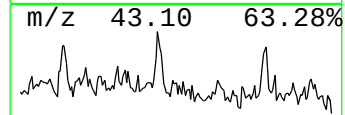
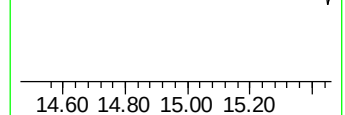
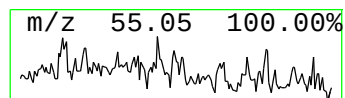
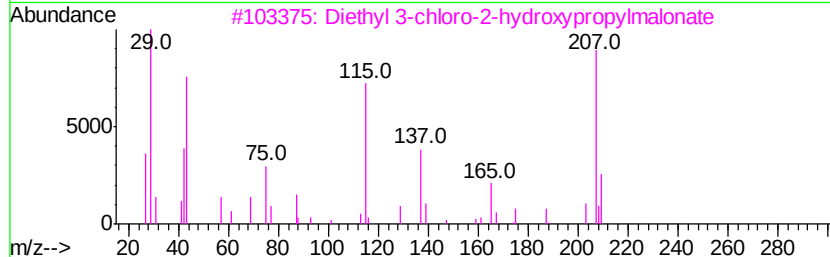
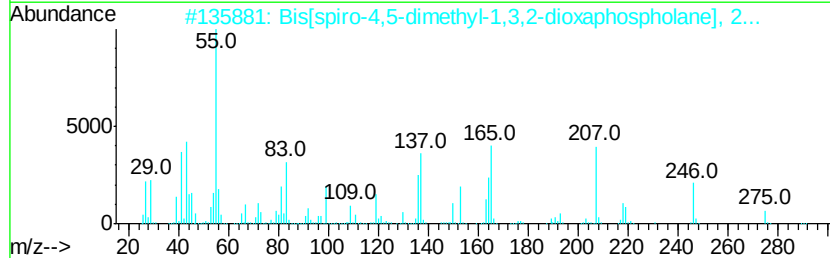
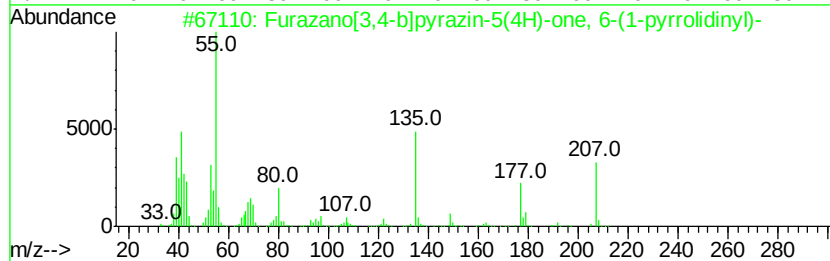
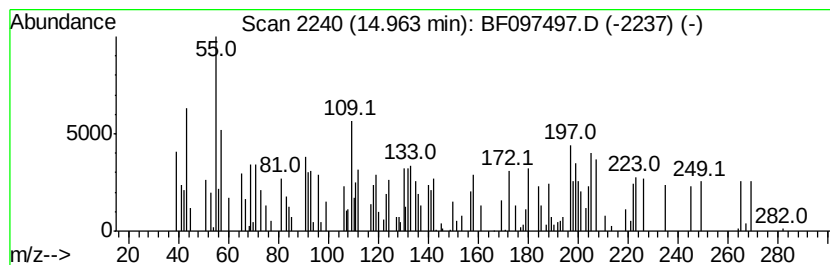
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Peak Number 6 unknown14.96 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.47 ng	43957	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Furazano[3,4-b]pyrazin-5(4H)-one...	207	C8H9N5O2	332099-72-6	10
2		Bis[spiro-4,5-dimethyl-1,3,2-dio...	290	C14H27O4P	1000150-50-8	9
3		Diethyl 3-chloro-2-hydroxypropyl...	252	C10H17ClO5	1000222-74-8	6
4		2,6-Lutidine, 3,5-dichloro-4-cyc...	289	C13H17Cl2NS	1000252-29-1	2
5		Cyclohexane, 1,1'-(2-propyl-1,3-...	250	C18H34	055030-21-2	1



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MW-1-080217

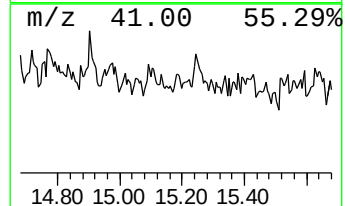
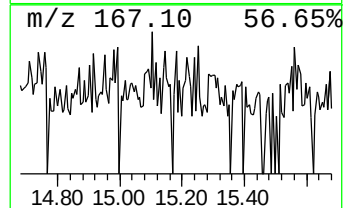
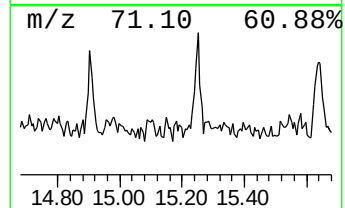
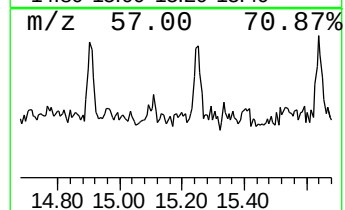
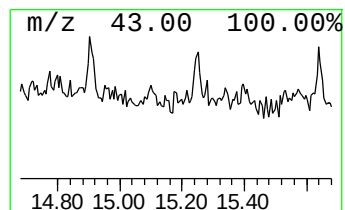
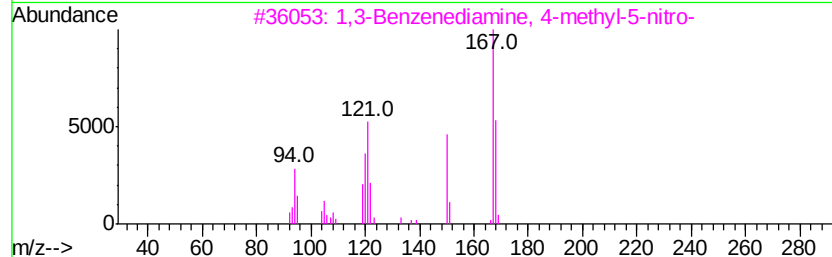
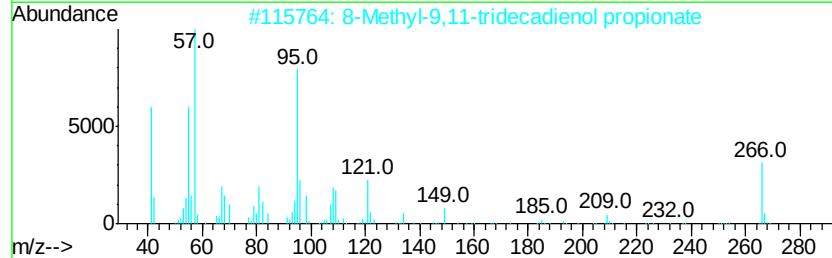
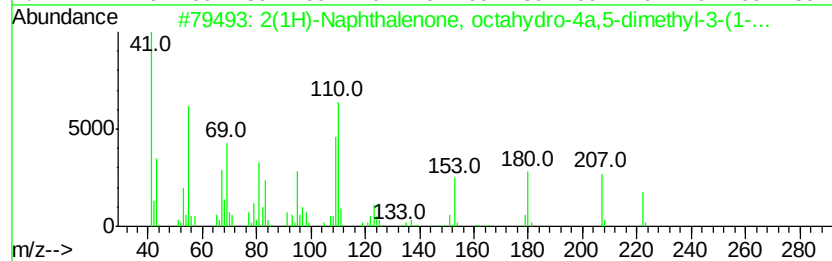
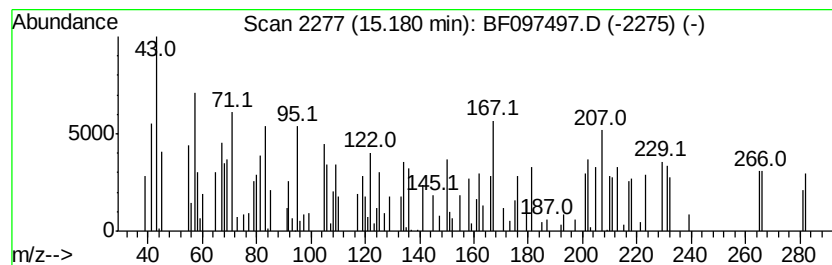
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.18 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.18	2.22 ng	39482	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(1H)-Naphthalenone, octahydro-4...	222	C15H26O	055332-04-2	10
2		8-Methyl-9,11-tridecadienol prop...	266	C17H30O2	1000130-96-9	9
3		1,3-Benzenediamine, 4-methyl-5-n...	167	C7H9N3O2	006629-29-4	9
4		N-(2,2-Diphenylethyl)-2,2-dimeth...	281	C19H23NO	1000211-18-7	9
5		1H-Pyrrole-2-carboxylic acid, 3,...	167	C9H13NO2	002199-44-2	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080817\
Data File : BF097497.D
Acq On : 9 Aug 2017 4:38
Operator : SJ/JU
Sample : I4604-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1-080217

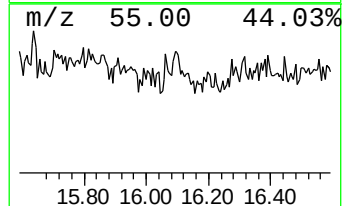
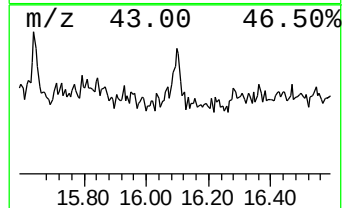
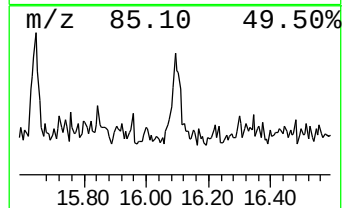
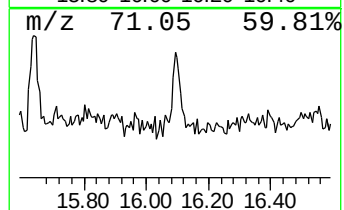
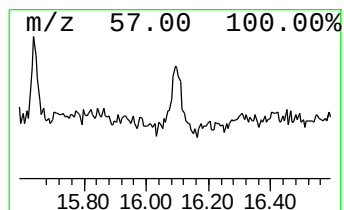
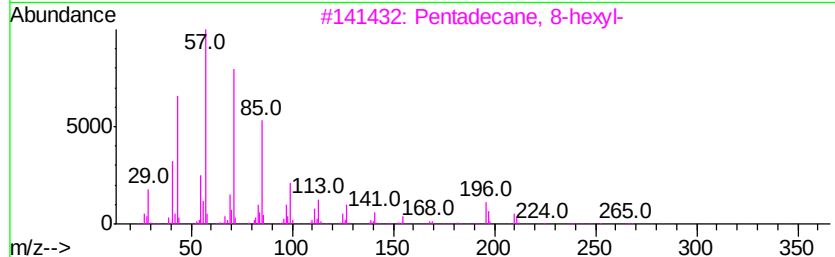
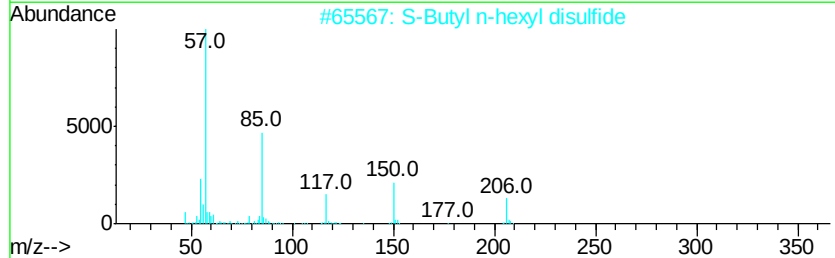
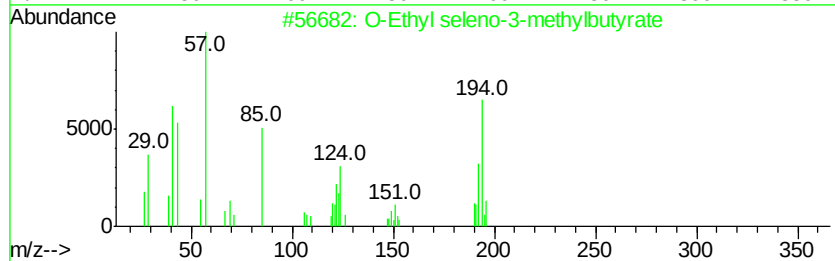
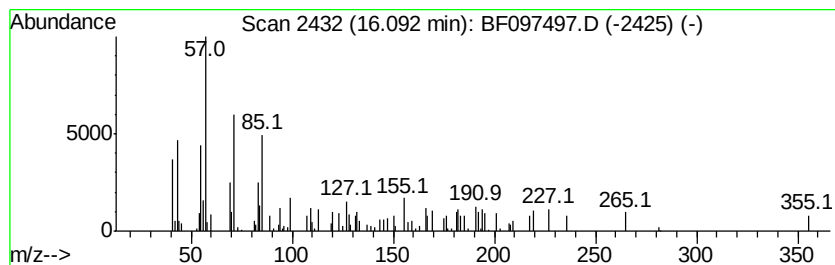
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.09 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	3.44 ng	61164	Perylene-d12	14.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	O-Ethyl seleno-3-methylbutyrate	194	C7H14OSe	1000074-76-5	22
2		S-Butyl n-hexyl disulfide	206	C10H22S2	169611-28-3	10
3		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	10
4		1,3,2-Dioxaphospholane, 2-t-buty...	292	C12H21O6P	080043-97-6	9
5		3-Methylpyrazolobis(diethylboryl...	236	C12H26B2N2O	1000159-71-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080817\
Data File : BF097497.D
Acq On : 9 Aug 2017 4:38
Operator : SJ/JU
Sample : I4604-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1-080217

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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...	4.53	3.0	ng	81523	1	6.40	536208	20.0
unknown6.18	6.18	77.6	ng	2079910	1	6.40	536208	20.0
Dodecanoic acid	11.47	2.1	ng	49512	4	10.90	472417	20.0
unknown12.30	12.30	2.8	ng	63869	5	13.53	464270	20.0
unknown14.96	14.96	2.5	ng	43957	6	14.87	355235	20.0
unknown15.18	15.18	2.2	ng	39482	6	14.87	355235	20.0
unknown16.09	16.09	3.4	ng	61164	6	14.87	355235	20.0