

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
 Data File : BF124767.D
 Acq On : 26 Jul 2021 16:19
 Operator : JU/CG
 Sample : M3117-08
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NJ-CLEAN-8

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-BF072221.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124767.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	7	11	14	rBB	8691	9294	8.12%	1.156%
2	5.087	507	510	513	rBB	1793	1806	1.58%	0.225%
3	5.487	573	578	580	rBB	98763	94568	82.60%	11.764%
4	6.492	745	749	752	rBB	113106	97450	85.11%	12.122%
5	6.869	810	813	816	rBB	46621	33600	29.35%	4.180%
6	7.434	905	909	911	rBB	75897	64631	56.45%	8.040%
7	8.051	1011	1014	1019	rBB	19118	14046	12.27%	1.747%
8	8.151	1028	1031	1034	rBB	57490	45911	40.10%	5.711%
9	9.228	1210	1214	1217	rBV	155369	114494	100.00%	14.243%
10	9.910	1327	1330	1333	rBB	68835	50765	44.34%	6.315%
11	10.698	1460	1464	1467	rBB	74242	63782	55.71%	7.934%
12	11.392	1579	1582	1586	rBB	51534	45402	39.65%	5.648%
13	11.916	1668	1671	1673	rBB	10409	6904	6.03%	0.859%
14	12.604	1786	1788	1791	rBB	2400	1642	1.43%	0.204%
15	12.698	1802	1804	1806	rBB	3855	2163	1.89%	0.269%
16	12.833	1825	1827	1830	rBB	2137	1670	1.46%	0.208%
17	12.980	1848	1852	1855	rBV	106729	80421	70.24%	10.004%
18	13.886	2002	2006	2011	rBB3	3030	4256	3.72%	0.529%
19	14.033	2027	2031	2034	rBV	34926	28500	24.89%	3.545%
20	14.192	2056	2058	2063	rBB	1843	1637	1.43%	0.204%
21	14.498	2105	2110	2113	rBB2	1797	1951	1.70%	0.243%
22	14.804	2160	2162	2166	rVB	1460	1644	1.44%	0.205%
23	15.074	2205	2208	2211	rBV	2216	2320	2.03%	0.289%
24	15.145	2217	2220	2225	rBB2	2107	2336	2.04%	0.291%
25	15.380	2256	2260	2264	rBB	1522	1761	1.54%	0.219%
26	15.439	2267	2270	2274	rBB	1465	1478	1.29%	0.184%
27	15.509	2277	2282	2289	rBB2	23529	29449	25.72%	3.663%

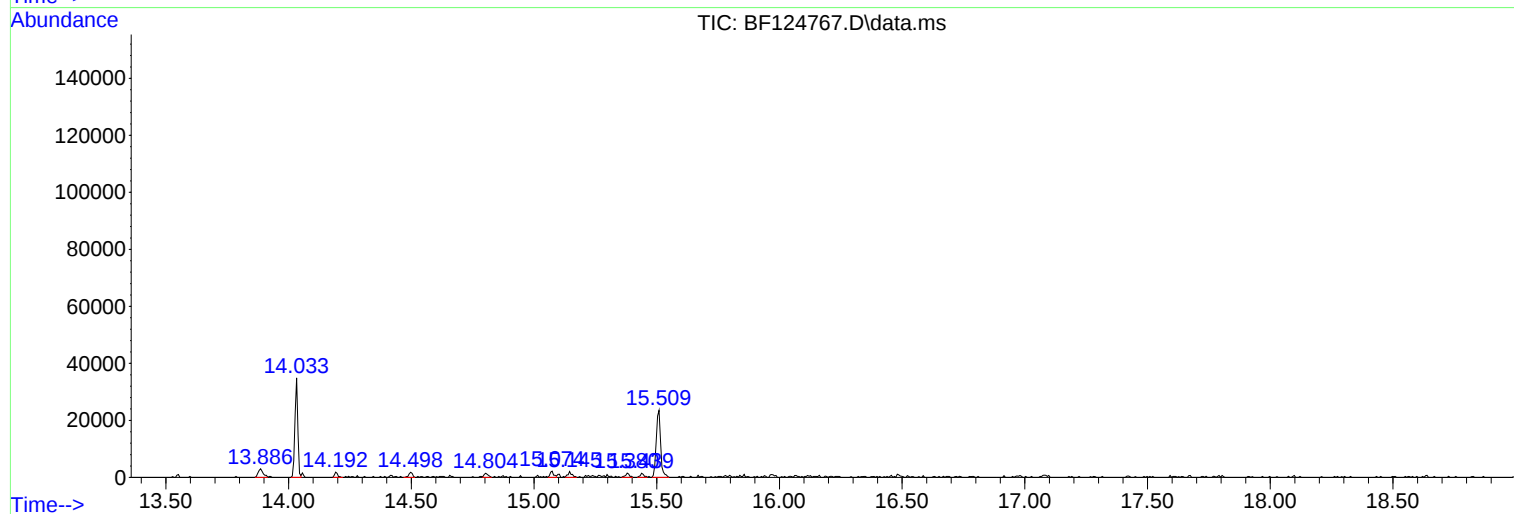
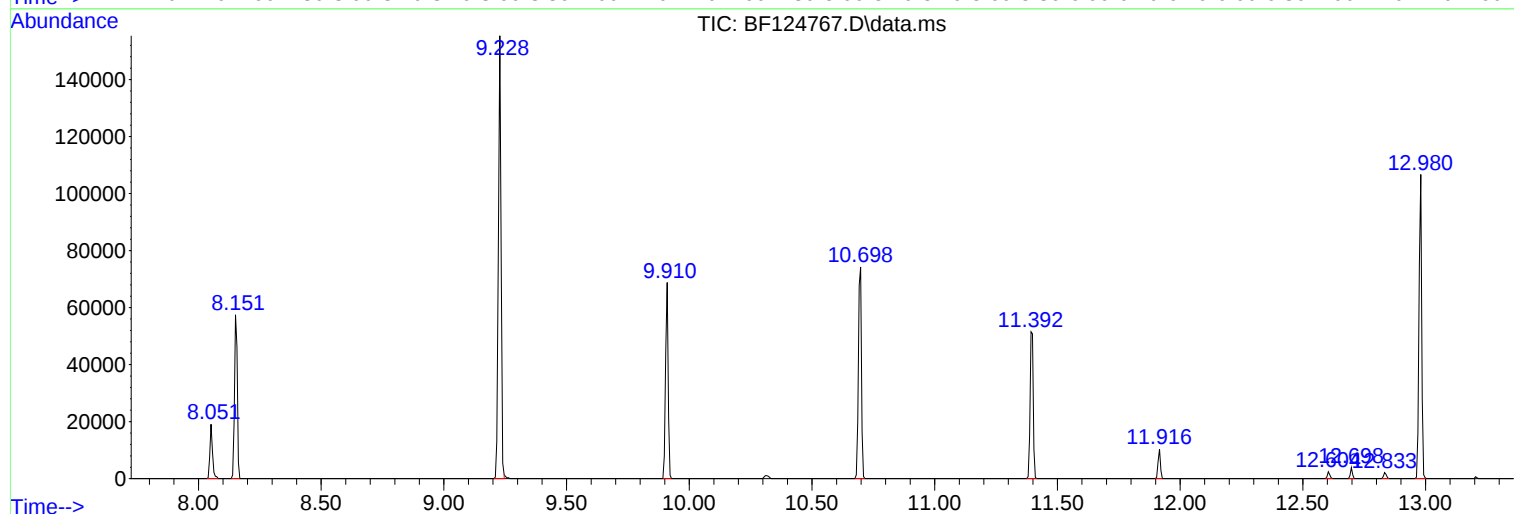
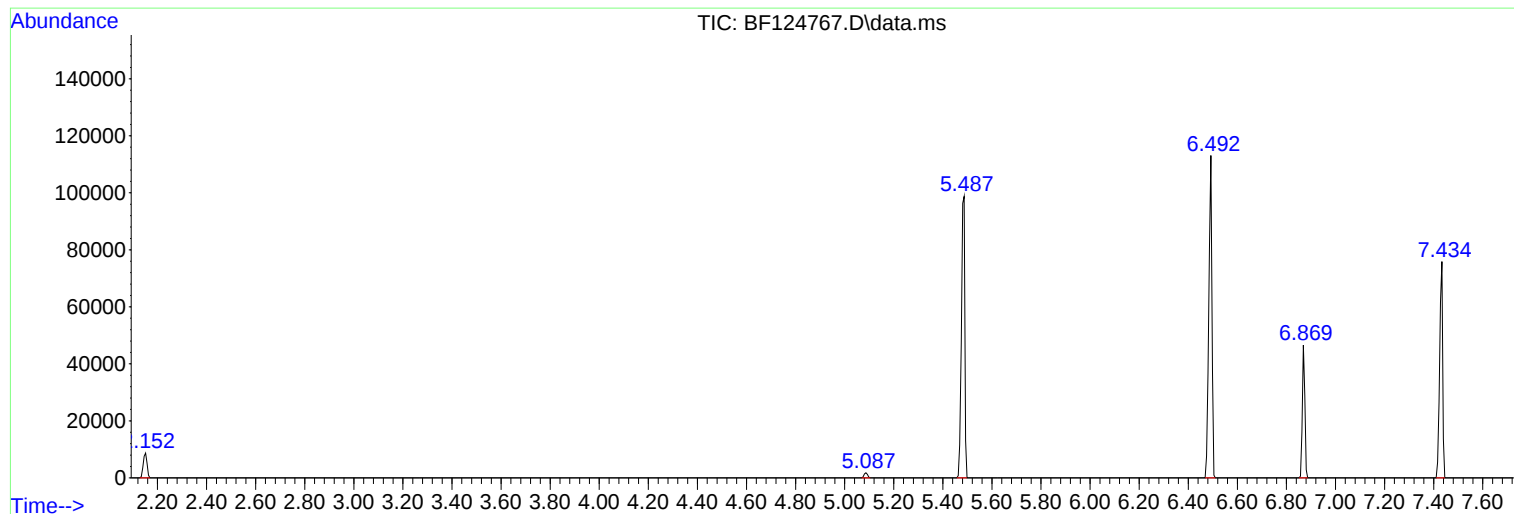
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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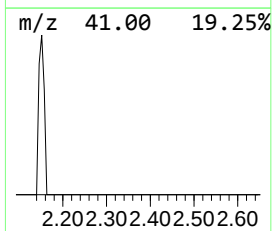
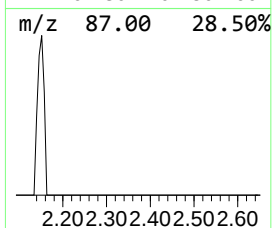
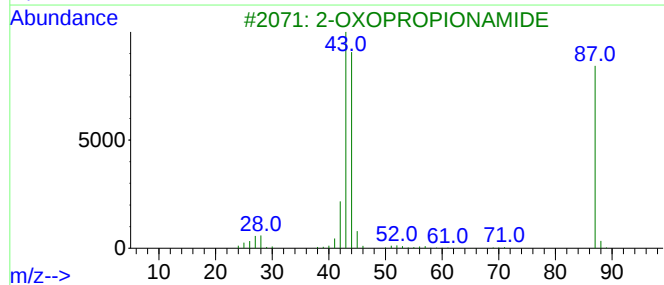
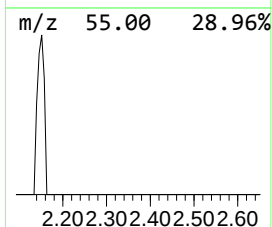
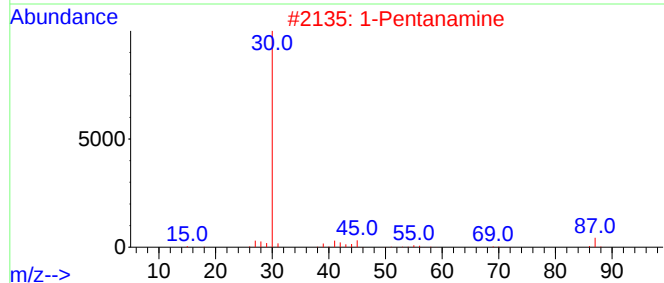
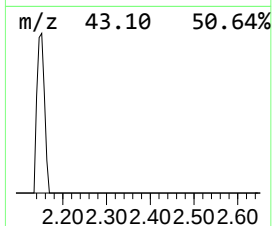
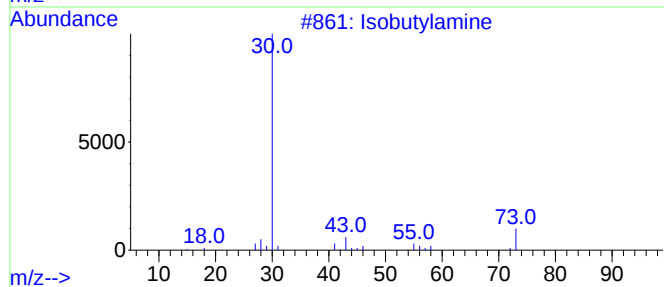
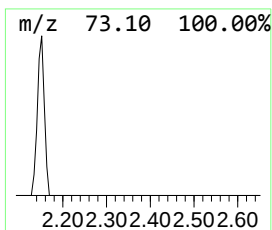
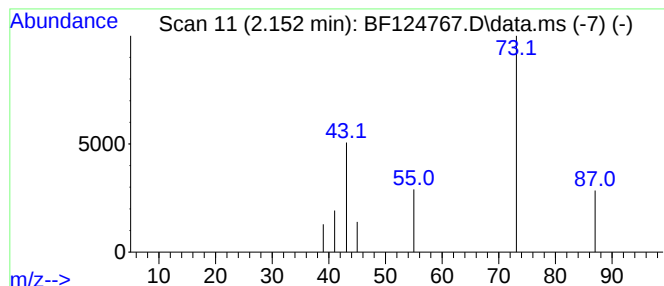
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.152 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	5.53 ng	9294	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutylamine	73	C4H11N	000078-81-9	5
2			1-Pentanamine	87	C5H13N	000110-58-7	4
3			2-OXOPROPIONAMIDE	87	C3H5NO2	000631-66-3	4
4			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	4
5			2-Pentanol, acetate	130	C7H14O2	000626-38-0	4



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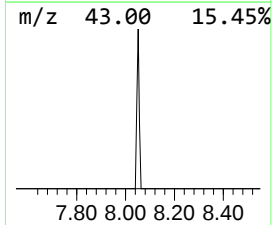
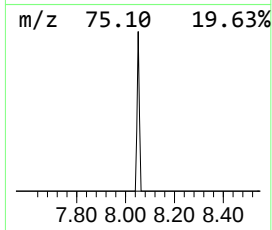
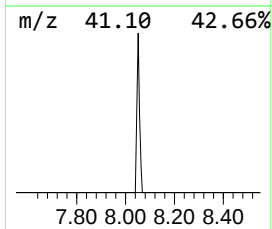
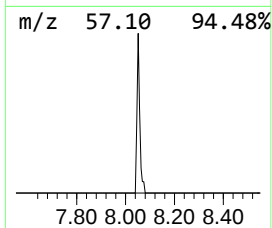
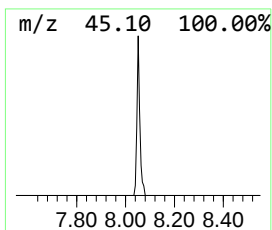
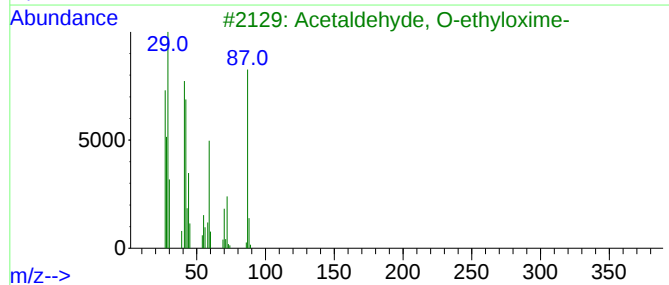
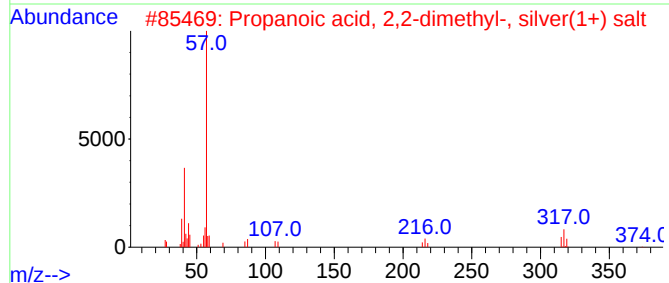
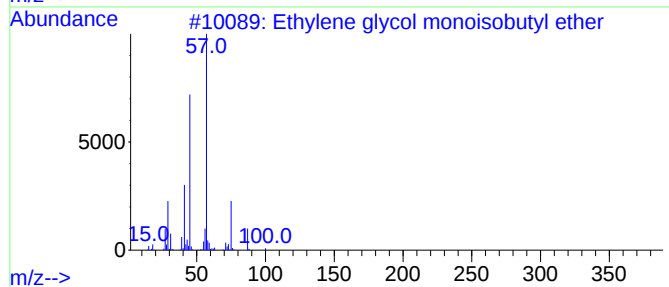
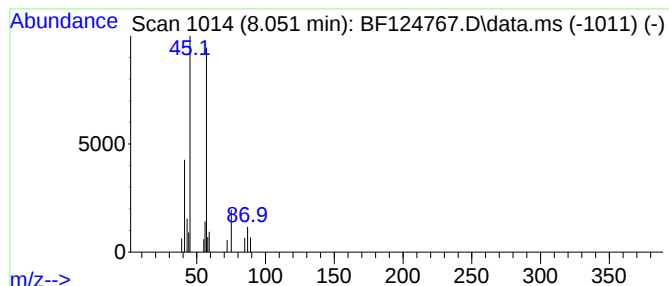
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Peak Number 2 unknown8.051 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	6.12 ng	14046	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	28
2			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	12
3			Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	9
4			1,3-Propanediol, 2-(hydroxymethy...	120	C5H12O3	000077-85-0	9
5			n-Butyl ether	130	C8H18O	000142-96-1	9



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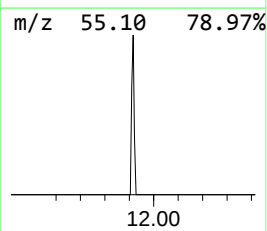
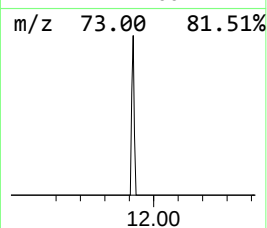
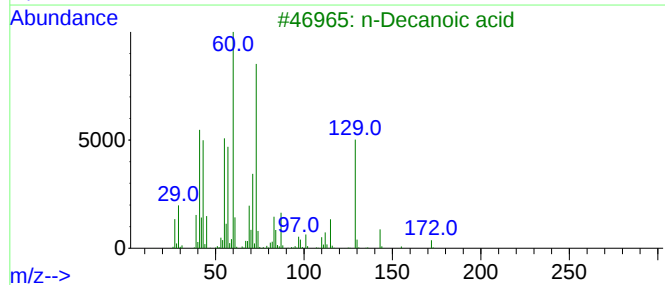
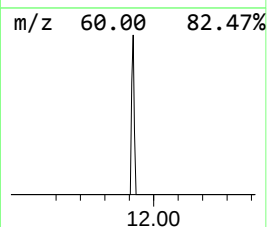
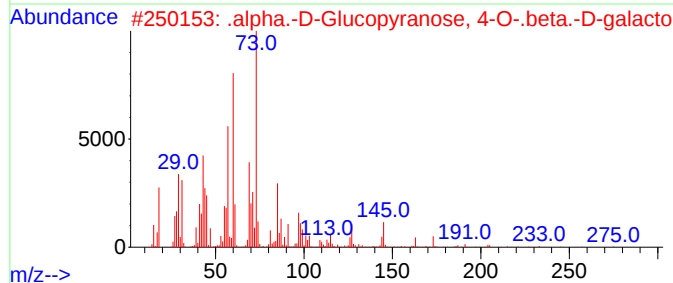
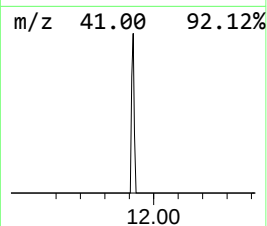
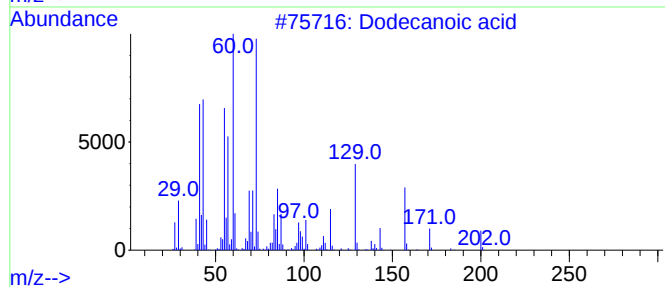
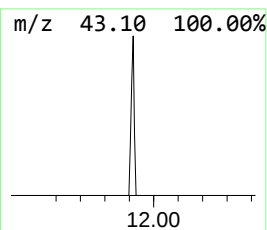
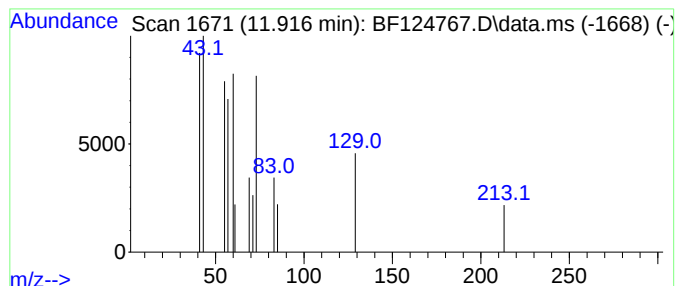
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Peak Number 3 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.04 ng	6904	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	64
2			.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	50
3			n-Decanoic acid	172	C10H20O2	000334-48-5	42
4			Undecanoic acid	186	C11H22O2	000112-37-8	36
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	28



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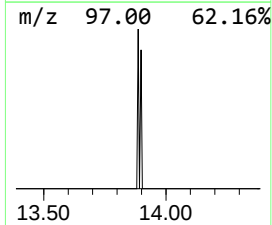
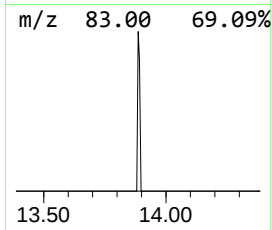
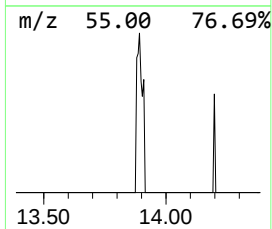
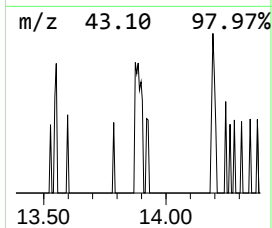
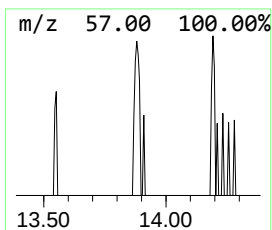
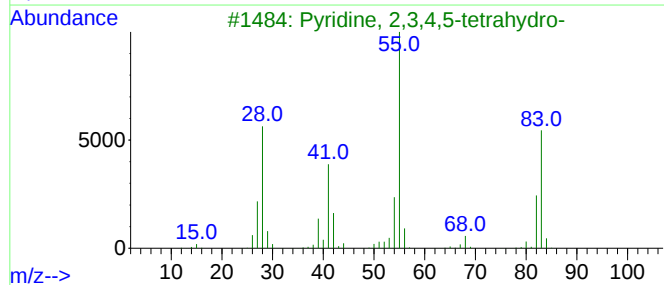
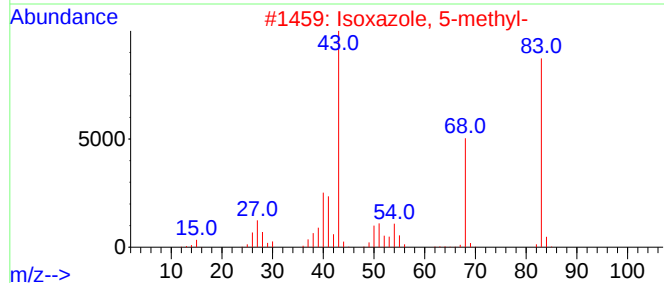
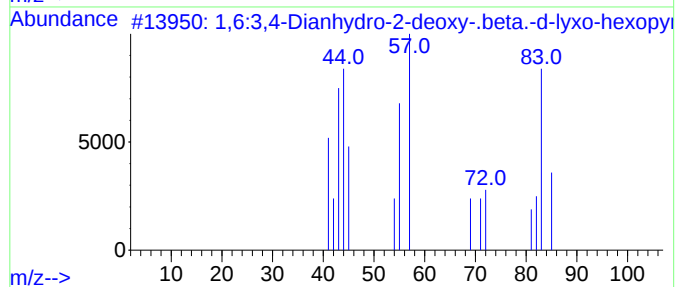
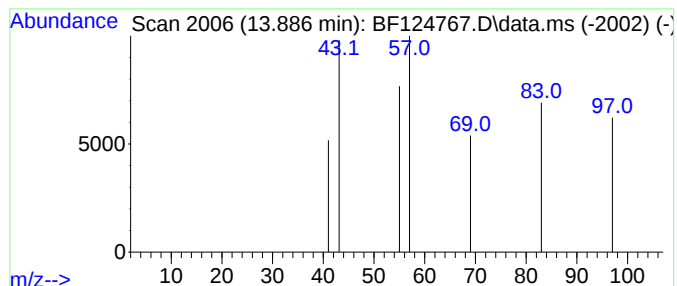
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Peak Number 4 unknown13.886 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	2.99 ng	4256	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6:3,4-Dianhydro-2-deoxy-.beta....	128	C6H8O3	050767-53-8	9		
2	Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	4		
3	Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	3		
4	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	3		
5	Cyclohexane, nitro-	129	C6H11NO2	001122-60-7	2		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.152	2.152	5.5	ng	9294	1	6.869	33600	20.0
unknown8.051	8.051	6.1	ng	14046	2	8.151	45911	20.0
Dodecanoic acid	11.916	3.0	ng	6904	4	11.398	45402	20.0
unknown13.886	13.886	3.0	ng	4256	5	14.033	28500	20.0