

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072221\
 Data File : BF124696.D
 Acq On : 22 Jul 2021 18:53
 Operator : JU/CG
 Sample : M3135-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-B

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: BF124696.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.157	8	12	15	rBB	9698	10681	6.18%	1.020%
2	5.092	507	511	514	rBB	4141	4697	2.72%	0.449%
3	5.481	573	577	580	rBB	132104	132098	76.37%	12.620%
4	6.492	743	749	751	rBB	126149	134746	77.90%	12.873%
5	6.869	810	813	816	rBB	41733	29947	17.31%	2.861%
6	7.428	904	908	911	rBB	93567	90425	52.28%	8.639%
7	8.051	1011	1014	1016	rBB	12329	9479	5.48%	0.906%
8	8.151	1027	1031	1034	rBB	55370	40464	23.39%	3.866%
9	9.227	1210	1214	1217	rBB	223544	172971	100.00%	16.525%
10	9.904	1326	1329	1332	rBB	58967	47366	27.38%	4.525%
11	10.692	1460	1463	1466	rBB	116612	99473	57.51%	9.503%
12	11.392	1579	1582	1585	rBB	61208	45635	26.38%	4.360%
13	11.915	1668	1671	1673	rBB	10795	7697	4.45%	0.735%
14	12.698	1802	1804	1806	rBB	4539	2790	1.61%	0.267%
15	12.980	1848	1852	1855	rBB	196184	158910	91.87%	15.181%
16	14.027	2027	2030	2033	rBB	38839	31057	17.96%	2.967%
17	15.498	2276	2280	2284	rBB	25915	28310	16.37%	2.705%

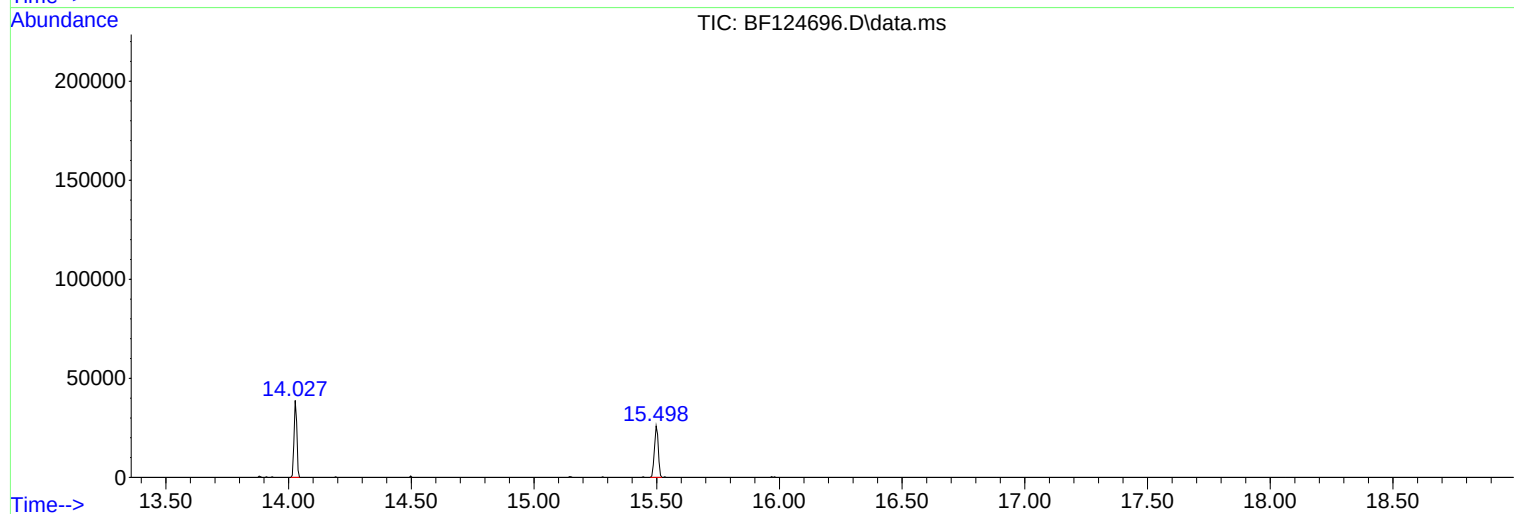
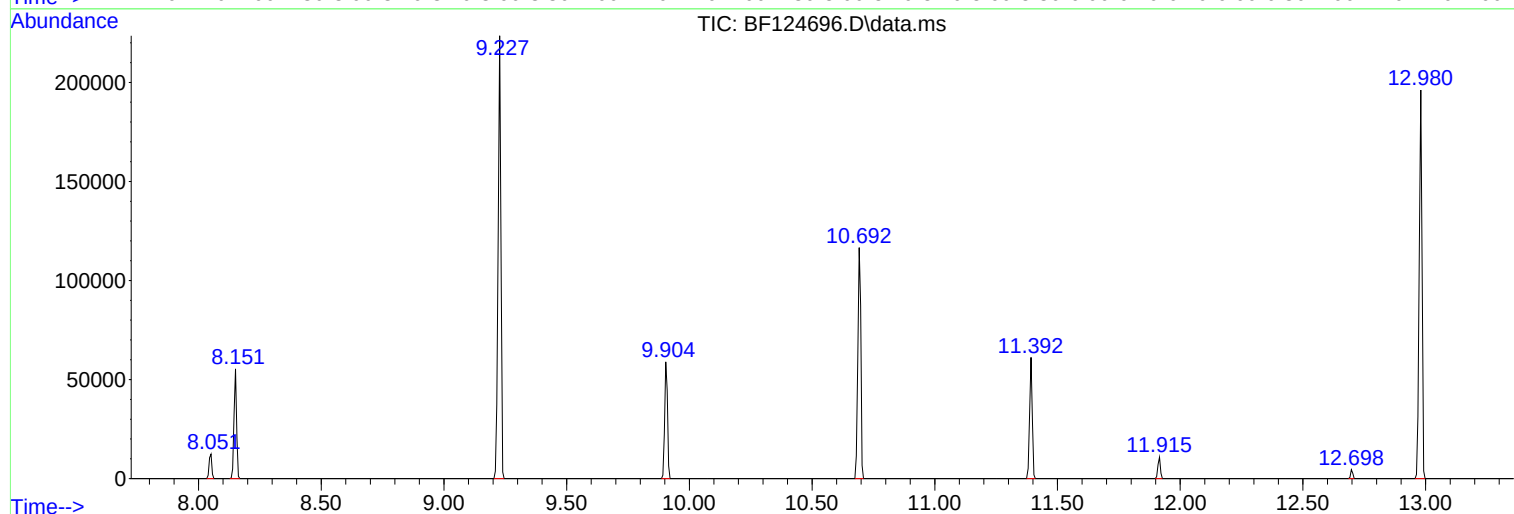
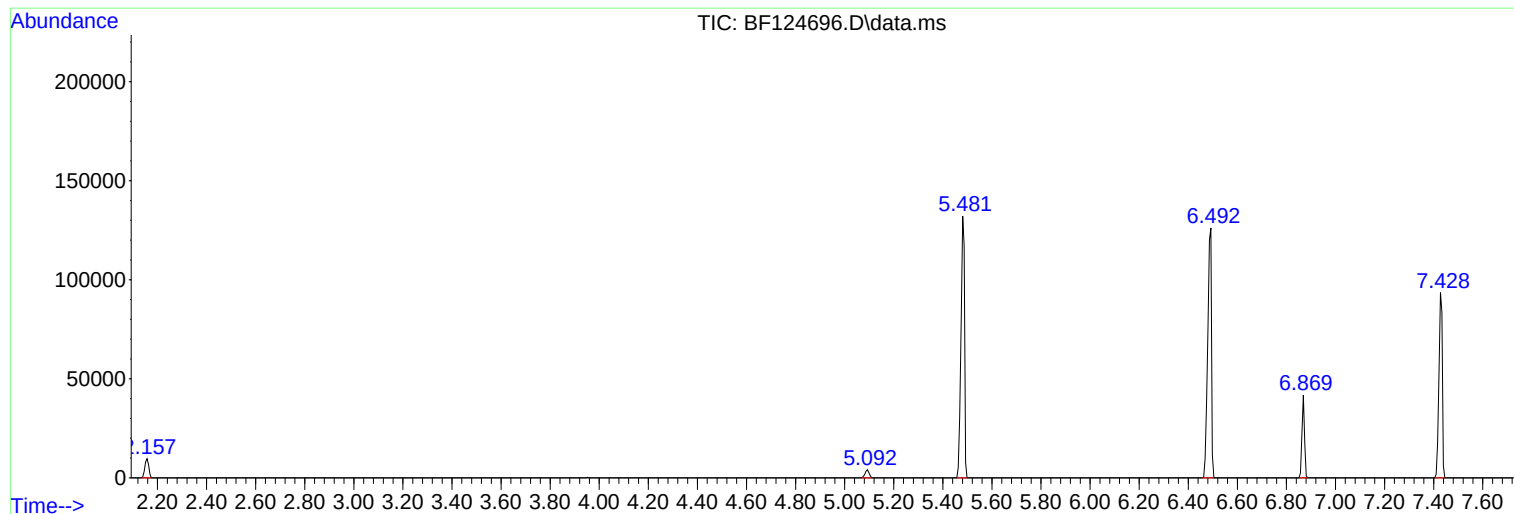
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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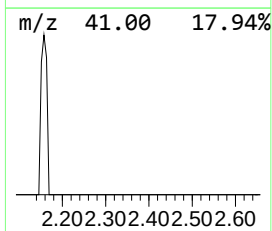
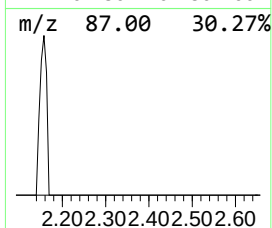
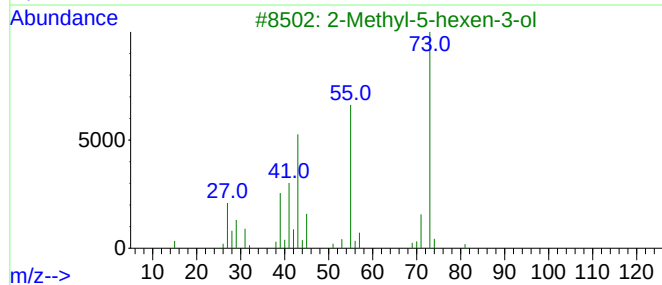
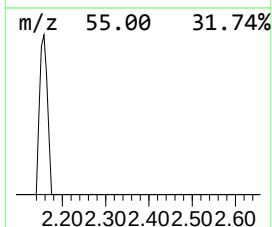
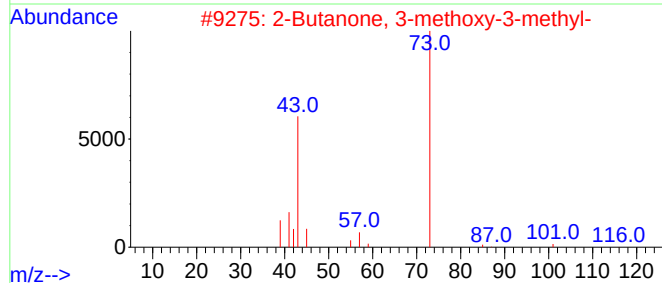
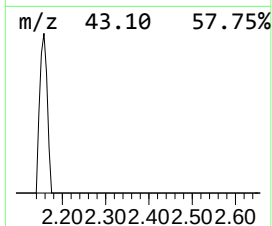
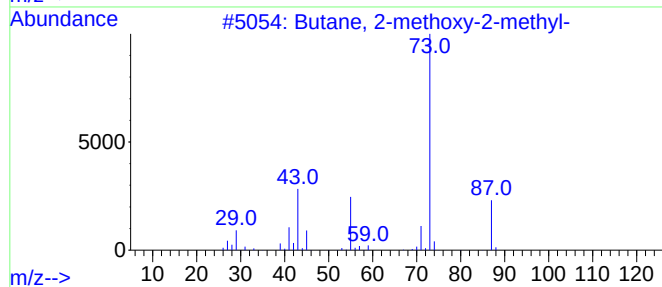
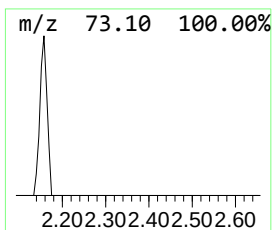
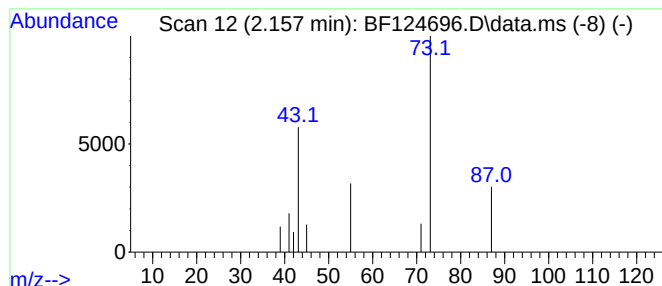
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	7.13 ng	10681	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	9
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
4			Isobutylamine	73	C4H11N	000078-81-9	5
5			N-Ethylformamide	73	C3H7NO	000627-45-2	5



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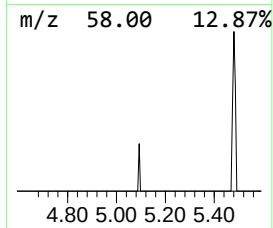
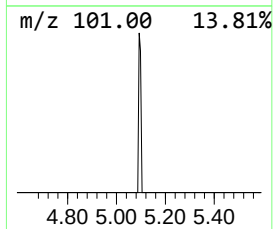
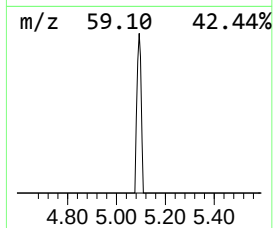
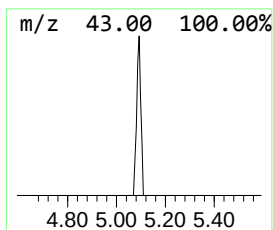
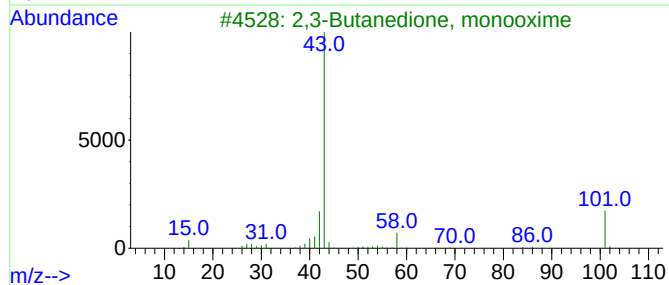
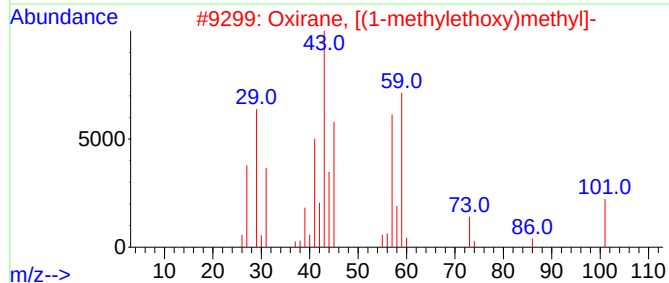
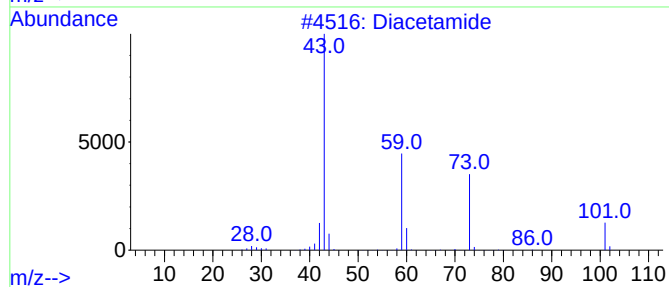
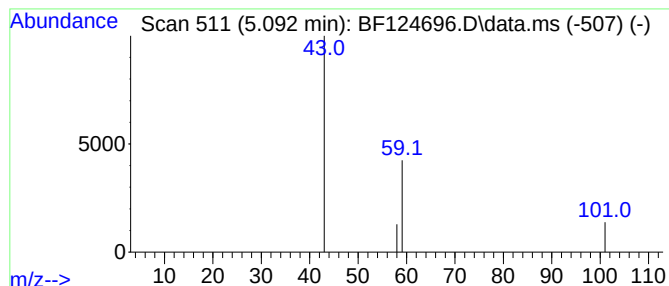
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.092 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.092	3.14 ng	4697	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diacetamide	101	C4H7NO2	000625-77-4	7
2			Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	4
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	3
4			Propylamine	59	C3H9N	000107-10-8	3
5			.alpha.-Amino-.gamma.-butyrolactone	101	C4H7NO2	001192-20-7	3



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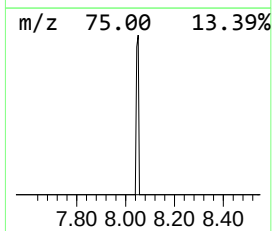
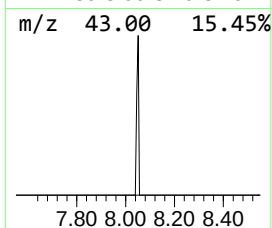
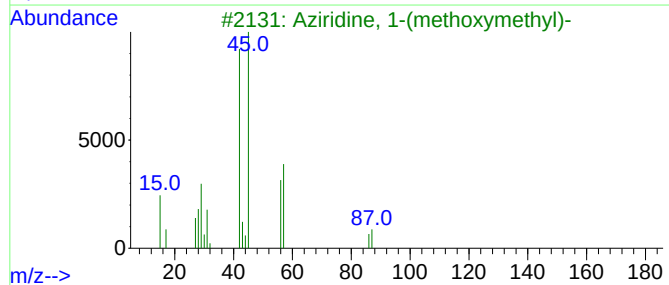
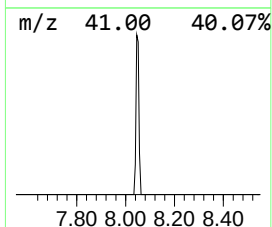
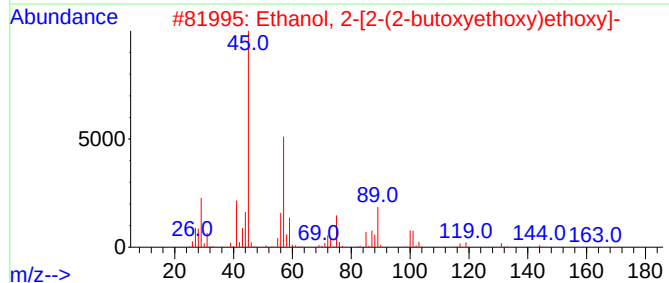
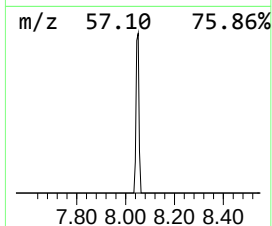
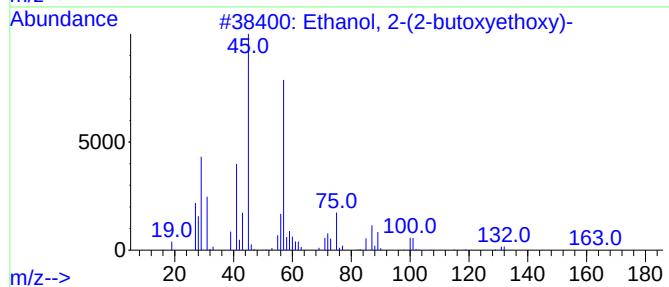
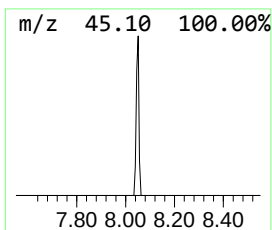
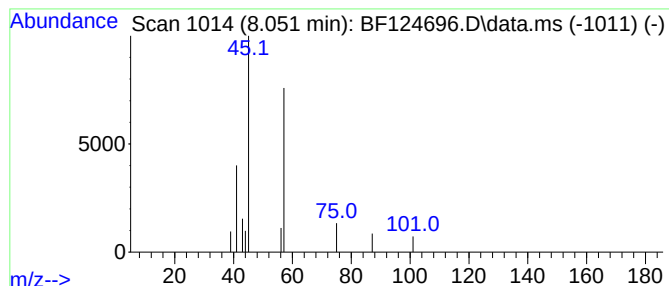
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Peak Number 3 unknown8.051 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	4.69 ng	9479	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	43
2			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	9
3			Aziridine, 1-(methoxymethyl)-	87	C4H9NO	001497-83-2	7
4			1-Hexanamine	101	C6H15N	000111-26-2	5
5			Neopentylamine	87	C5H13N	005813-64-9	5



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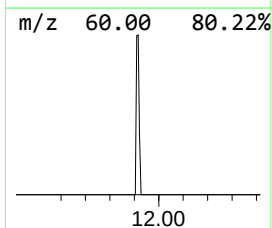
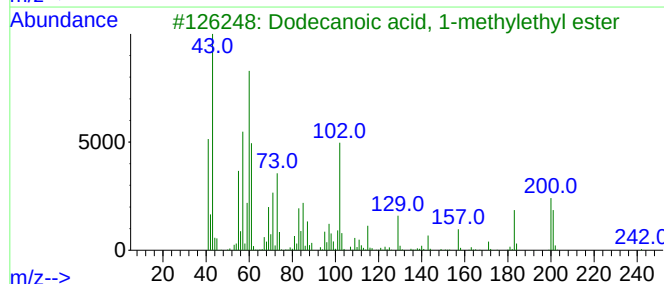
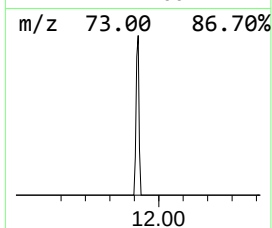
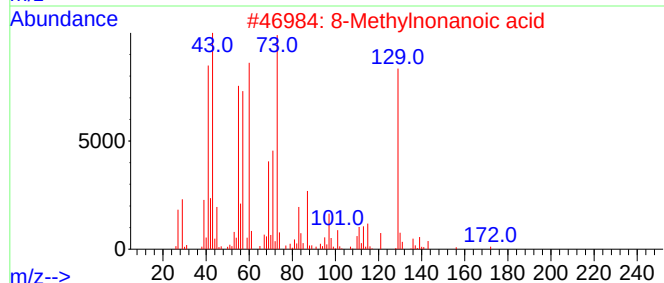
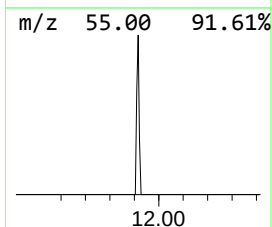
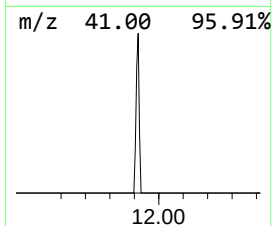
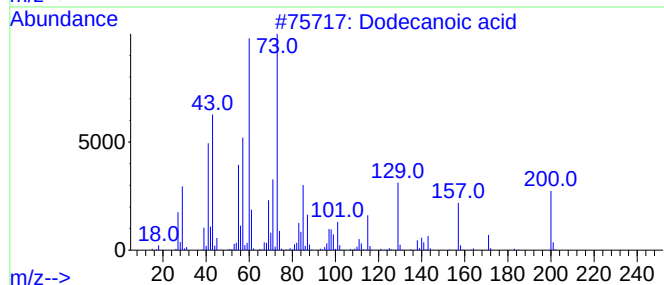
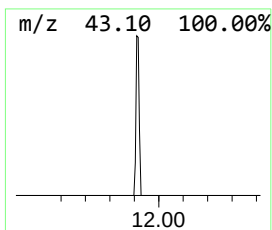
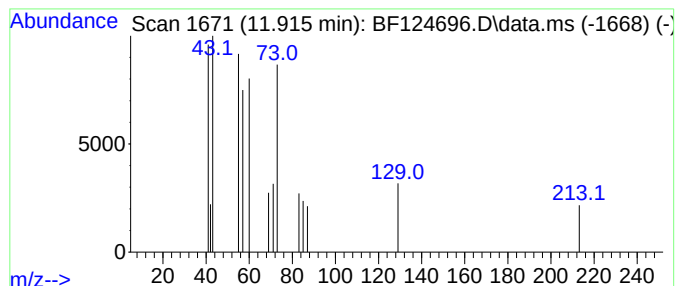
Instrument :
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Peak Number 4 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.916	3.37 ng	7697	Phenanthrene-d10	11.392	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	53
2	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	53
3	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	45
4	Undecanoic acid	186	C11H22O2	000112-37-8	45
5	n-Decanoic acid	172	C10H20O2	000334-48-5	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.157	7.1	ng	10681	1	6.869	29947	20.0
unknown5.092	5.092	3.1	ng	4697	1	6.869	29947	20.0
unknown8.051	8.051	4.7	ng	9479	2	8.151	40464	20.0
Dodecanoic acid	11.916	3.4	ng	7697	4	11.392	45635	20.0